Supporting Information

Carbon-Nitrogen Bond Formation Using Sodium Hexamethyldisilazide: Solvent-Dependent Reactivities and Mechanisms

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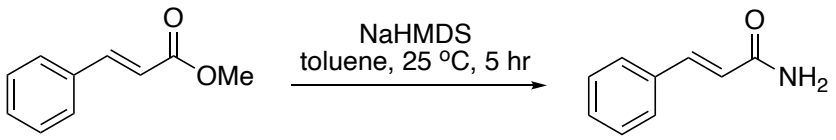
General Experimental Procedure

Reagents and solvents. NaHMDS and [^{15}N]NaHMDS were prepared as white crystalline solids. Toluene, hexanes, THF, MTBE, cyclopentane, 2,5-Me_2THF, and HMPA were distilled from blue or purple solutions containing sodium benzophenone ketyl. Substrates in Table 1 are all commercially available, and all products are either commercially available or available by literature procedures.

Synthesis of picolinamide : picolinamide (**4**). Solid sodium hexamethyldisilazide (NaHMDS, 165 mg, 0.9 mmol) was dissolved in 2.0 mL of DMEA at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 36 µL of methyl picolinate (**3**) (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 25 °C for 0.3 hr. DI water (1.0 mL) was added, and the resulting biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (80% ethyl acetate in hexanes) afforded picolinamide (**4**) as a white solid.

Synthesis of picolinimidamide : picolinimidamide (**7**). Solid sodium hexamethyldisilazide (NaHMDS, 165 mg, 0.9 mmol) was dissolved in 1.5 mL of THF at 25 °C. 1.5 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 36 µL methyl picolinate (**3**) (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 50 °C for 0.3 hr. DI water (1.0 mL) was then added. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 1 hr. Saturated NaOH solution was then added until pH = 12. Mixture was partitioned between water (1.0 mL) and chloroform (4.0 mL). The aqueous layer was separated and extracted further with three 4.0 mL portions of chloroform. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated to afford picolinimidamide (**7**) as a yellow oil.

Synthesis of cinnamamide 2



Solid sodium hexamethyldisilazide (NaHMDS, 110 mg, 0.6 mmol) was dissolved in 2.0 mL of toluene at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar, containing 50 mg of methyl cinnamate **1**(0.30 mmol). The reaction was stirred at 25 °C for 5 hr. DI water (1.0 mL) was added, and the resulting biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (50% ethyl acetate in hexanes) afforded 35 mg (73%) of product **2** as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.7 (d, J = 15.7 Hz, 1H), 7.5 (dd, J = 6.6, 3.0 Hz, 2H), 7.4 (q, J = 3.1 Hz, 3H), 6.5 (d, J = 15.7 Hz, 1H), 5.8 (s, 1H), 5.73 (s, 1H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 167.9, 142.6, 134.6, 130.1, 129.0, 128.0, 119.6.

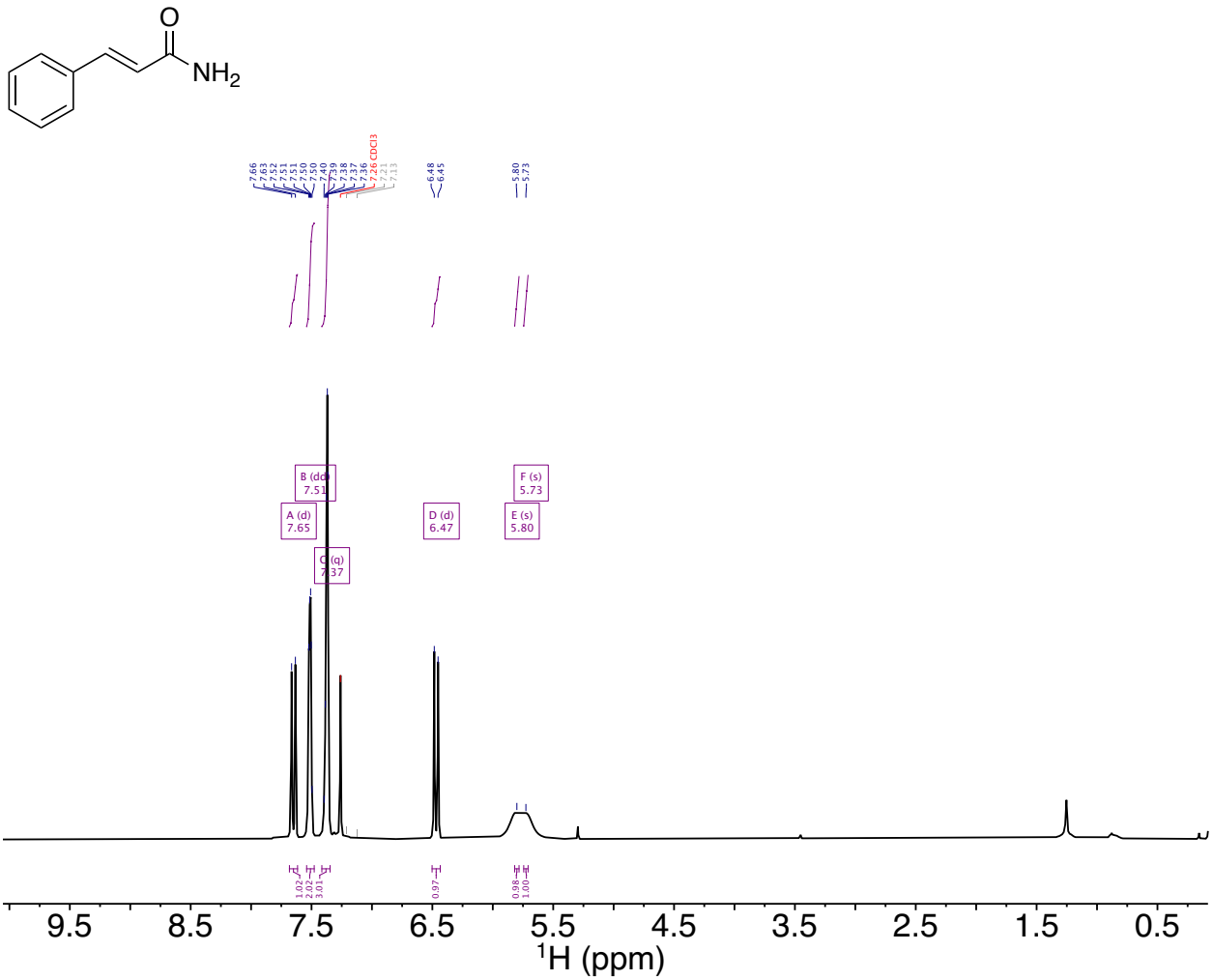


Figure S1. ^{1}H NMR spectrum of cinnamamide **2** in $CDCl_3$ w/ 0.05% TMS at 25 °C.

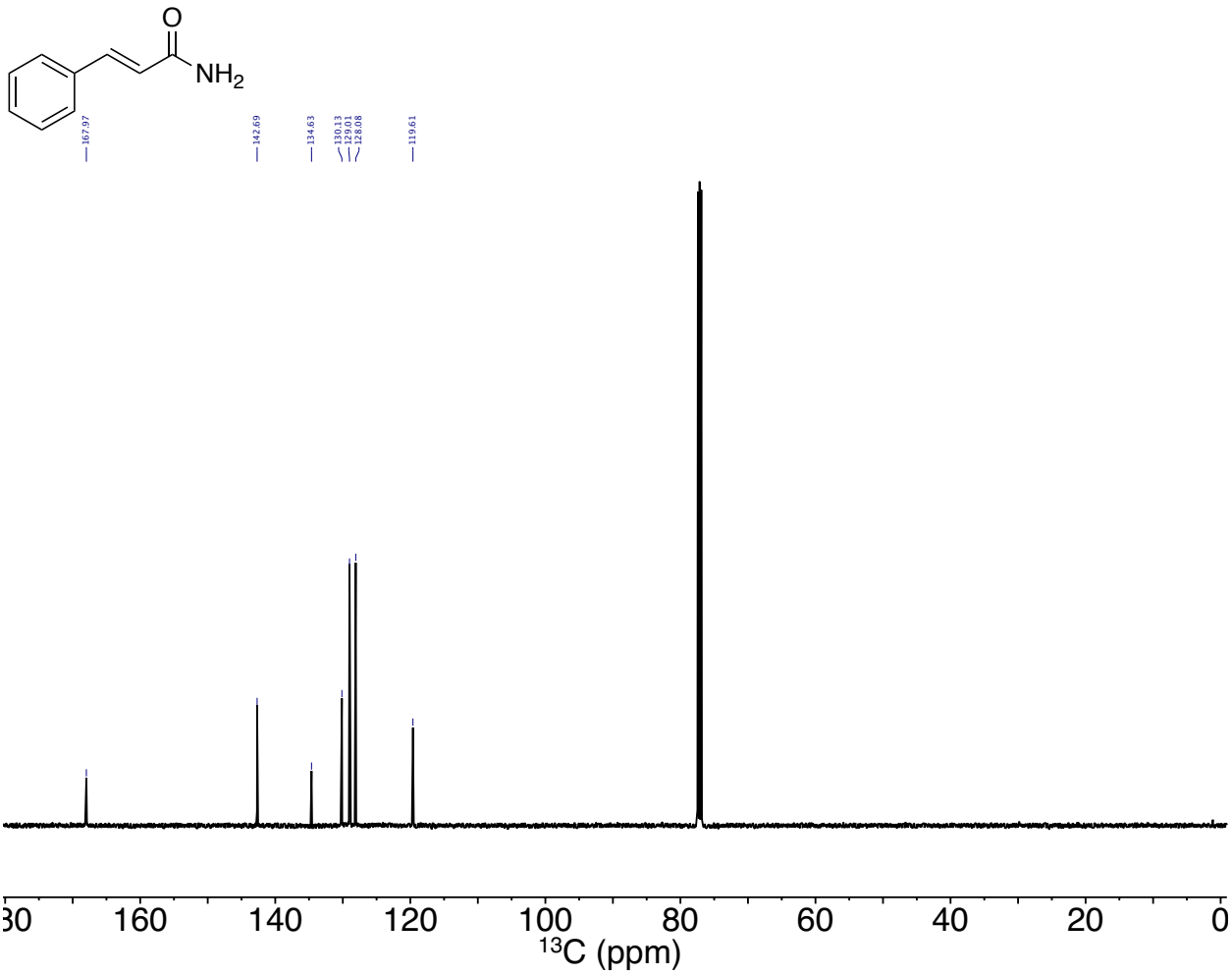
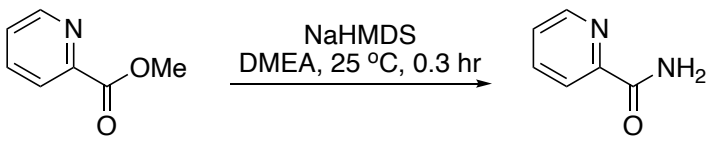


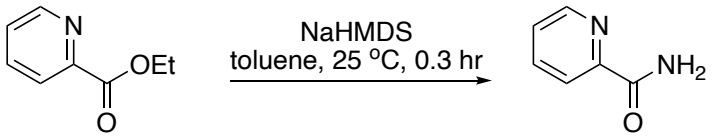
Figure S2. ^{13}C NMR spectrum of cinnamamide **2** in $CDCl_3$ w/ 0.05% TMS at 25 °C.

Synthesis of picolinamide 4 (a)



Solid sodium hexamethyldisilazide (NaHMDS, 165 mg, 0.9 mmol) was dissolved in 2.0 mL of DMEA at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 36 µL of methyl picolinate **3** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 25 °C for 0.3 hr. DI water (1.0 mL) was added, and the resulting biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (80% ethyl acetate in hexanes) afforded 39 mg (95%) of product picolinamide **4** as a white solid.

Synthesis of picolinamide 4 (b)



Solid sodium hexamethyldisilazide (NaHMDS, 165 mg, 0.90 mmol) was dissolved in 2.0 mL of toluene at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 34 µL of ethyl picolinate **5** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 25 °C for 0.3 hr. DI water (1.0 mL) was added, and the resulting biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (80% ethyl acetate in hexanes) afforded 37 mg (90%) of product picolinamide **4** as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.6 (d, J = 4.6 Hz, 1H), 8.2 (d, J = 7.8 Hz, 1H), 7.9 (s, 1H), 7.8 (td, J = 7.7, 1.8 Hz, 1H), 7.4 (dd, J = 7.6, 4.8 Hz, 1H), 6.2 (s, 1H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 166.9, 145.6, 148.3, 137.3, 126.5, 122.4.

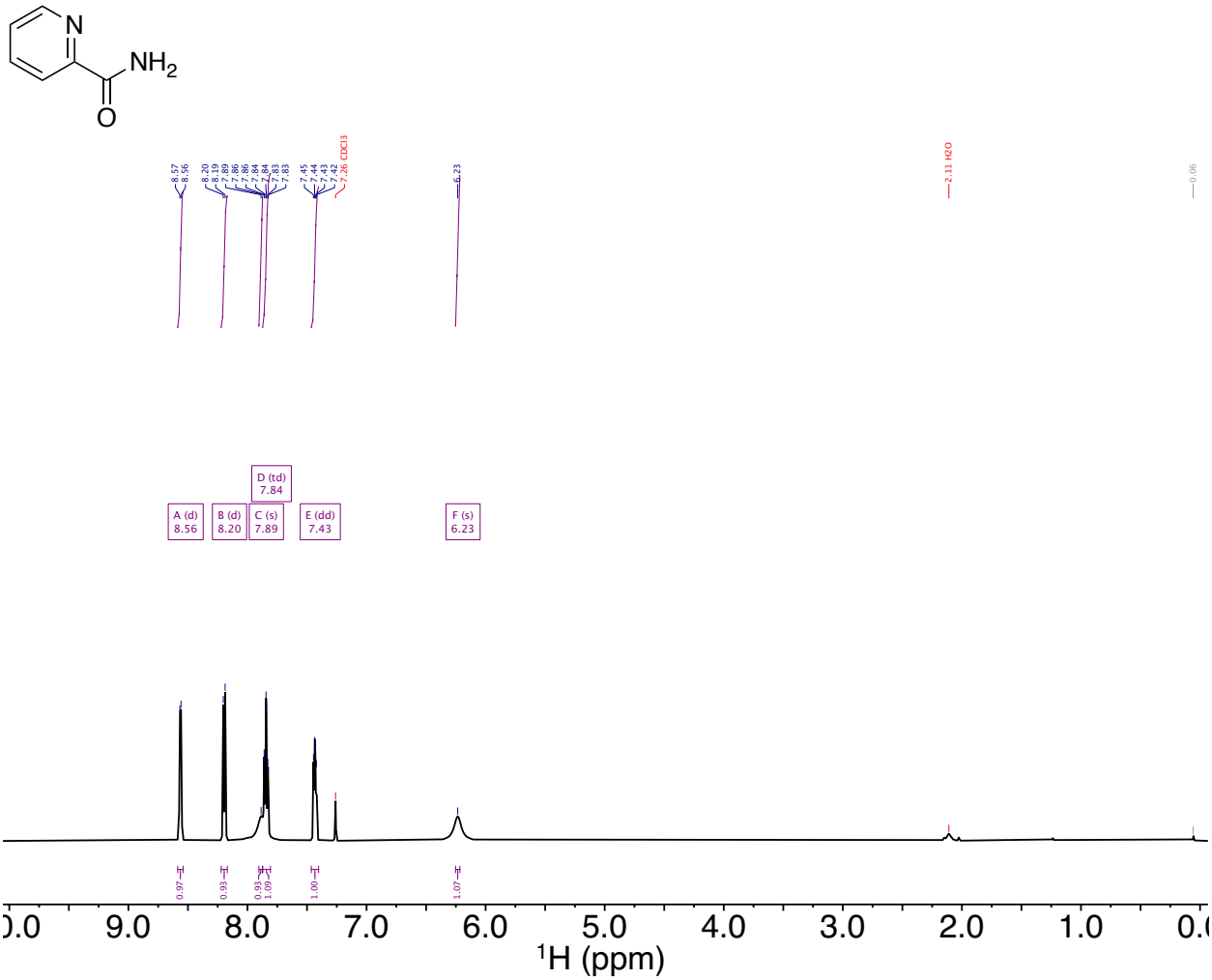


Figure S3. ^{1}H NMR spectrum of picolinamide **4** in $CDCl_3$ at 25 °C.

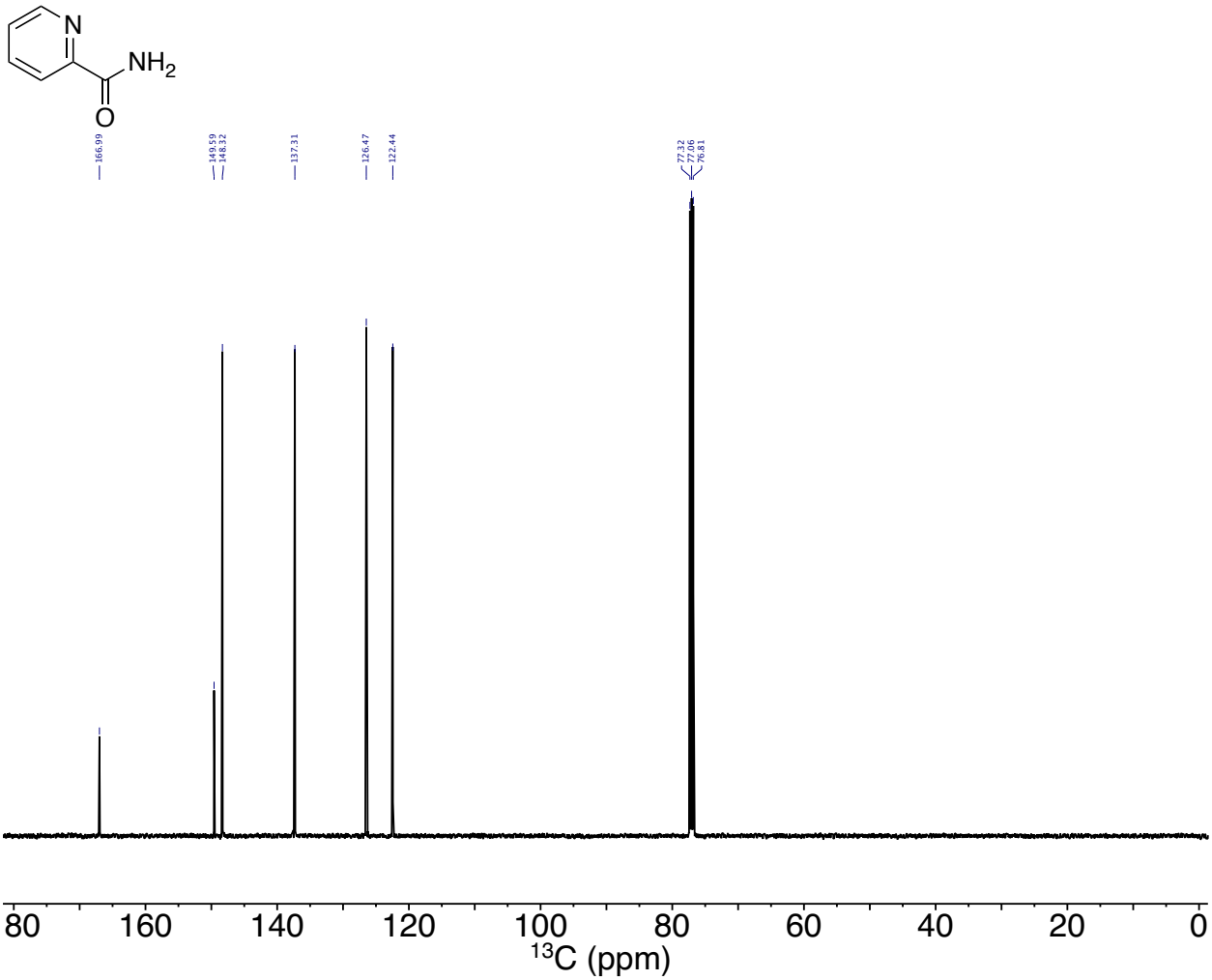
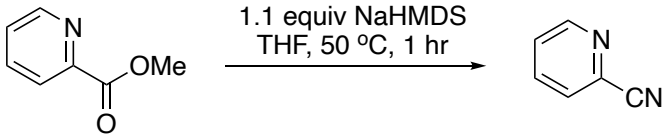


Figure S4. ^{13}C NMR spectrum of picolinamide **4** in $CDCl_3$ at 25 °C.

Synthesis of picolinonitrile 6



Solid sodium hexamethyldisilazide (NaHMDS, 330 mg, 1.8 mmol) was dissolved in 3.0 mL of THF at 25 °C. 0.60 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 36.5 µL of methyl picolinate **3** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 25 °C for 0.3 hr. DI water (1.0 mL) was added, and the resulting biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers

were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (20% ethyl acetate in hexanes) afforded 37 mg (90%) of product picolinonitrile **6** as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.7 (dt, *J* = 4.9, 1.4 Hz, 1H), 7.8 (td, *J* = 7.8, 1.7 Hz, 1H), 7.7 (dt, *J* = 7.8, 1.2 Hz, 1H), 7.5 (ddd, *J* = 7.8, 4.8, 1.2 Hz, 1H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 151.2, 137.1, 134.0, 128.6, 127.0, 117.2.

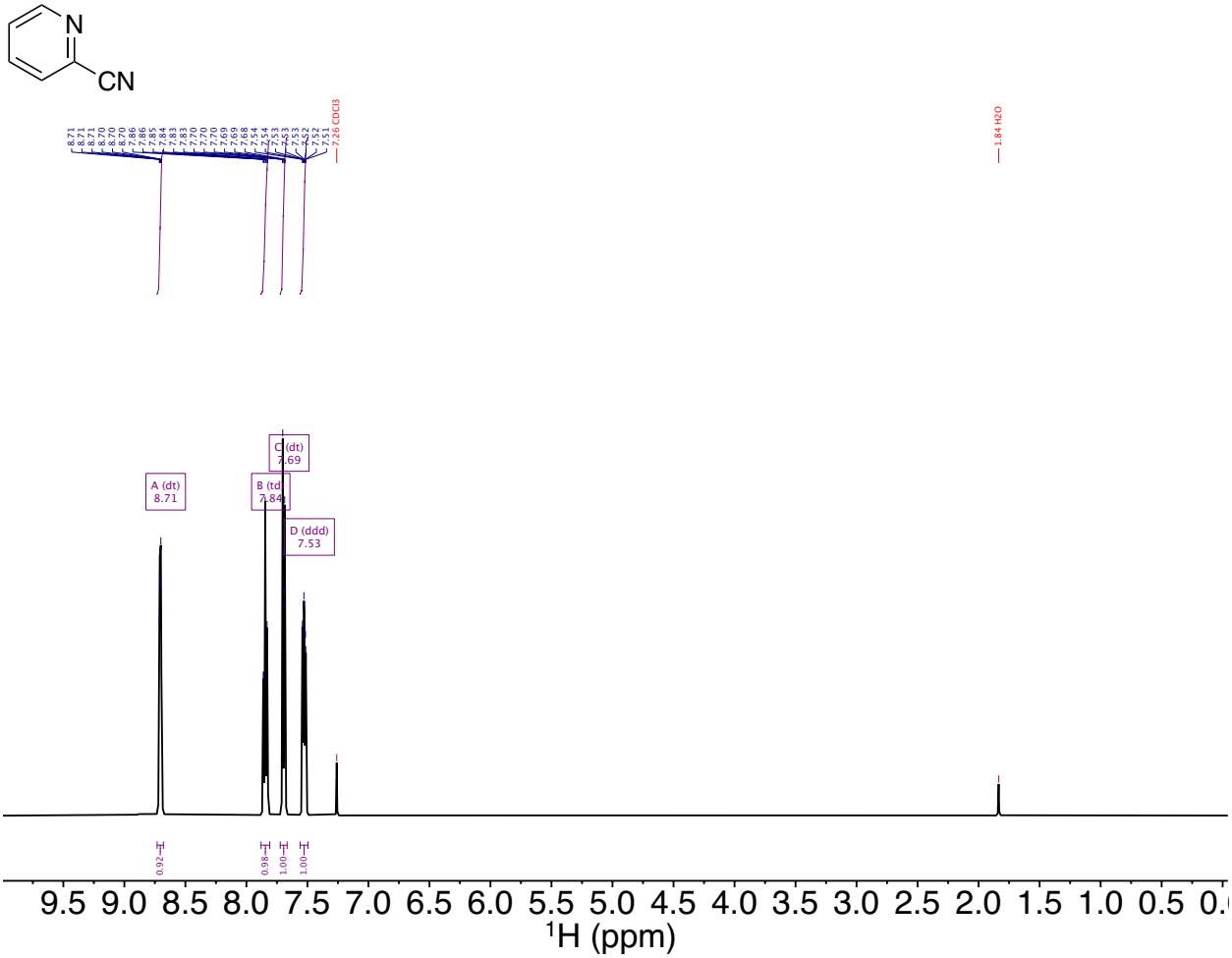


Figure S5. ^{1}H NMR spectrum of picolinonitrile **6** in $CDCl_3$ at 25 °C.

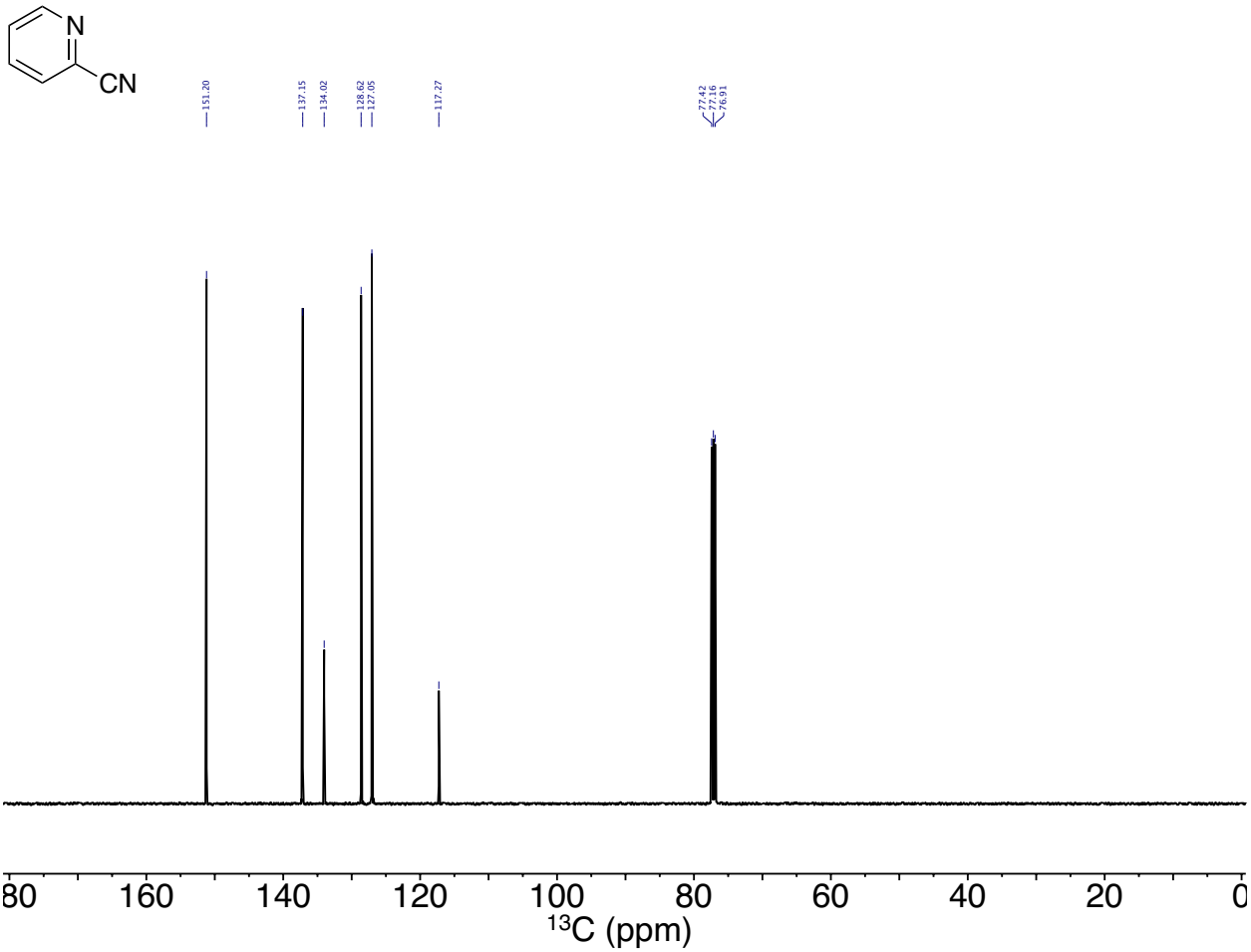
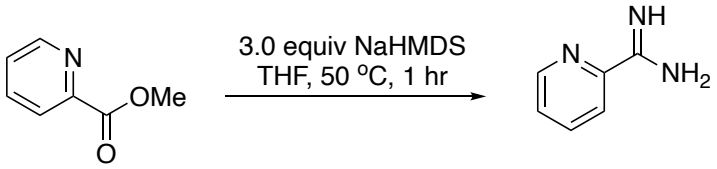


Figure S6. ^{13}C NMR spectrum of picolinonitrile **6** in $CDCl_3$ at 25 °C.

Synthesis of picolinimidamide 7



Solid sodium hexamethyldisilazide (NaHMDS, 330 mg, 1.8 mmol) was dissolved in 3.0 mL of THF at 25 °C. 1.5 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 36.5 µL of methyl picolinate **3** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 50 °C for 0.3 hr. Rotavap THF. DI water (1.0 mL) was then added. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 1 hr. Saturated NaOH solution was then added until pH = 12. Mixture was partitioned between water (1.0 mL) and chloroform (4.0 mL). The aqueous layer was separated and extracted further with three 4.0 mL portions of chloroform. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated to afford product 33.4 mg (92%) of product picolinimidamide **7** as an off-white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.6 (m, 1H), 8.1 (d, *J* = 7.9 Hz, 1H), 7.8 (td, *J* = 7.7, 1.8 Hz, 1H), 7.4 (dd, *J* = 7.5, 4.9 Hz, 1H), 5.9 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 161.1, 150.8, 148.4, 137.0, 125.2, 120.8.

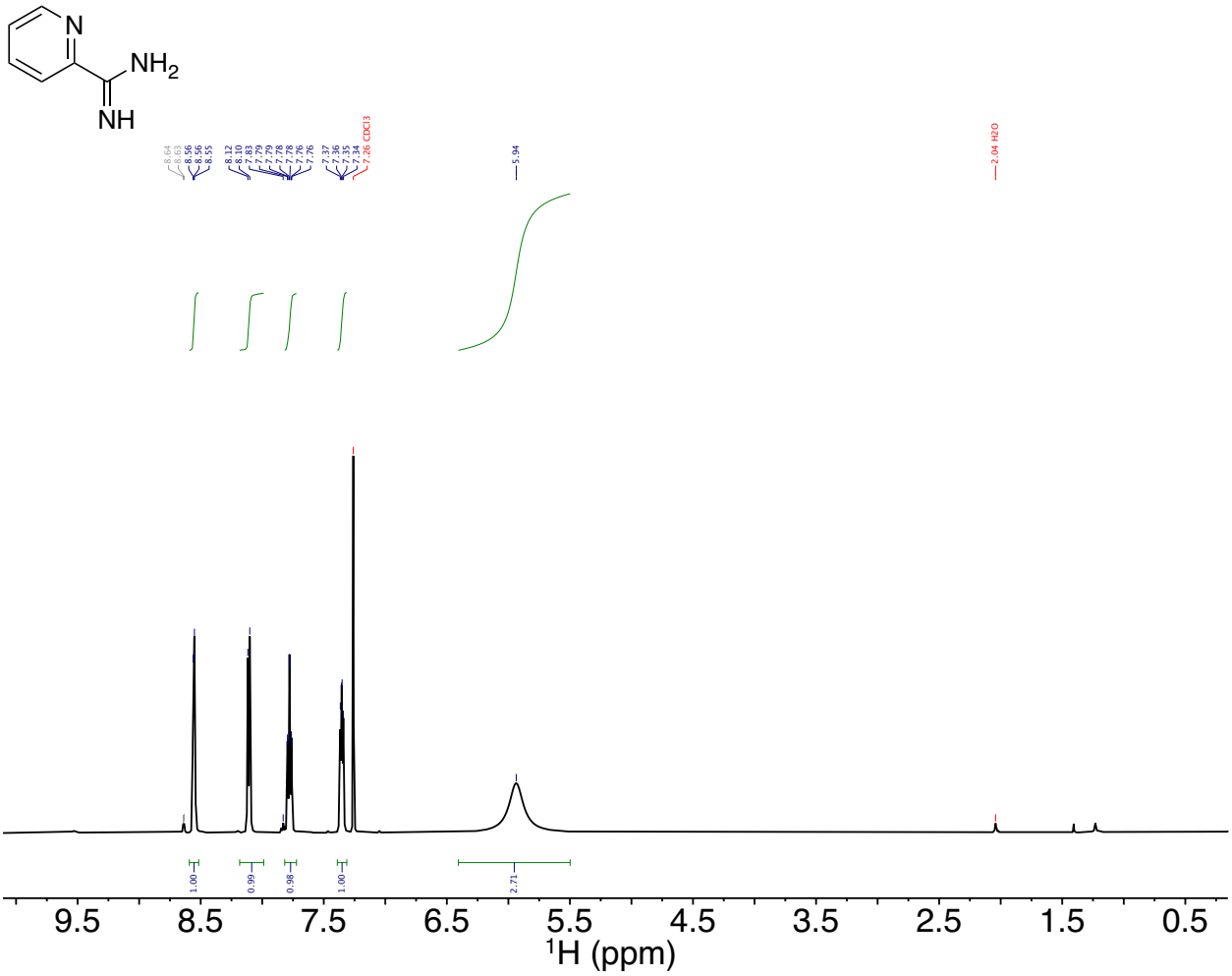


Figure S7. ^{1}H NMR spectrum of picolinimidamide **7** in $CDCl_3$ at 25 °C.

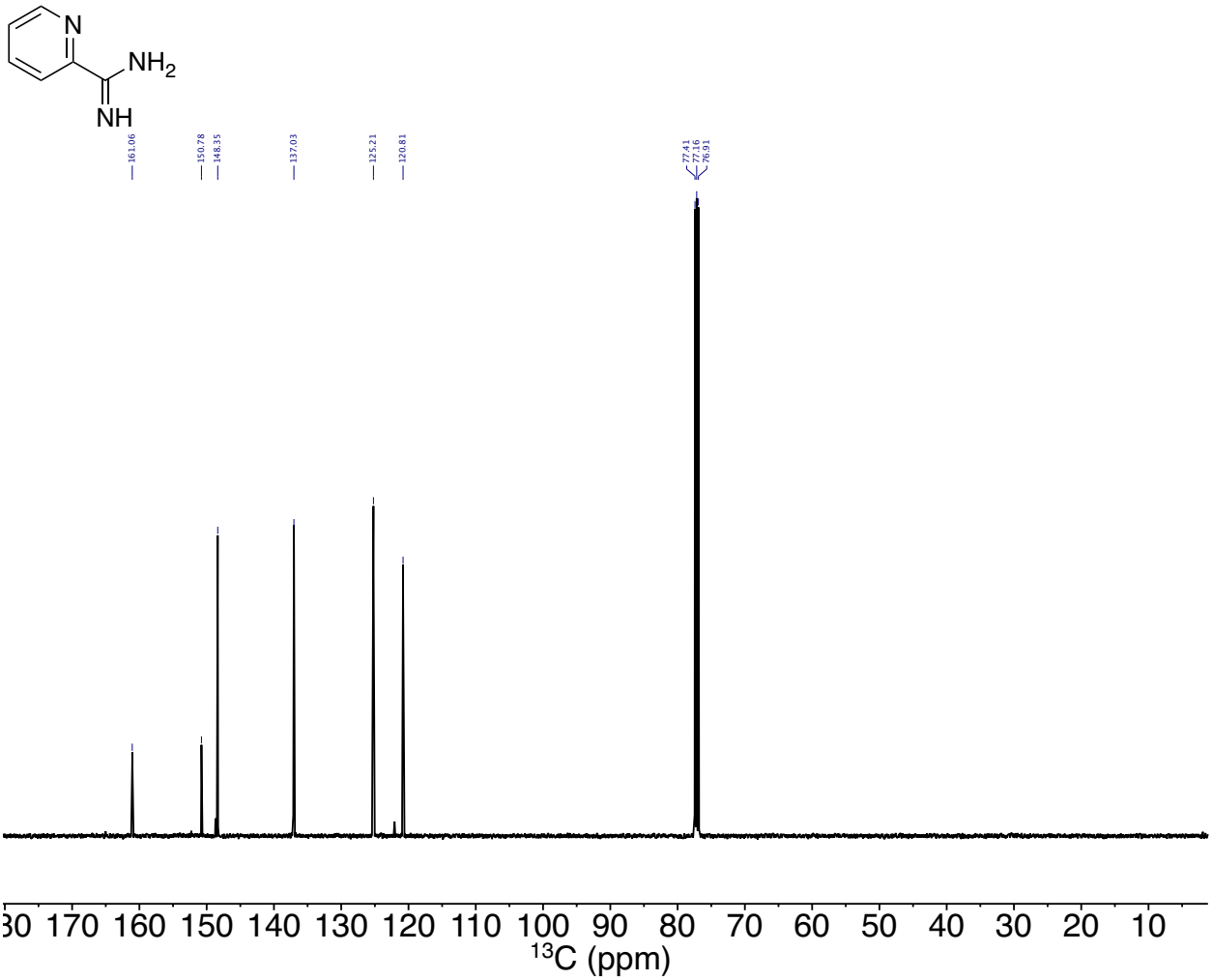
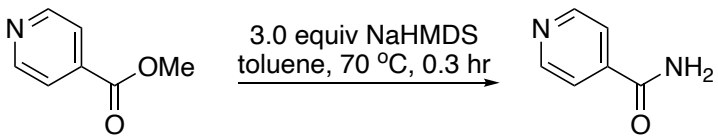


Figure S8. ^{13}C NMR spectrum of picolinimidamide **7** in $CDCl_3$ at 25 °C.

Synthesis of isonicotinamide 9



Solid sodium hexamethyldisilazide (NaHMDS, 165 mg, 0.9 mmol) was dissolved in 2.0 mL of toluene at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar, containing 42 mg of methyl isonicotinate (**8**) (0.30 mmol). The reaction was stirred at 70 °C for 0.3 hr. DI water (1.0 mL) was added, and the resulting biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (80% ethyl acetate in hexanes) afforded 31 mg (85%) of product isonicotinamide **9** as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.9 (s, 2H), 7.1 (s, 2H).

$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 167.5, 148.9, 140.7, 121.1.

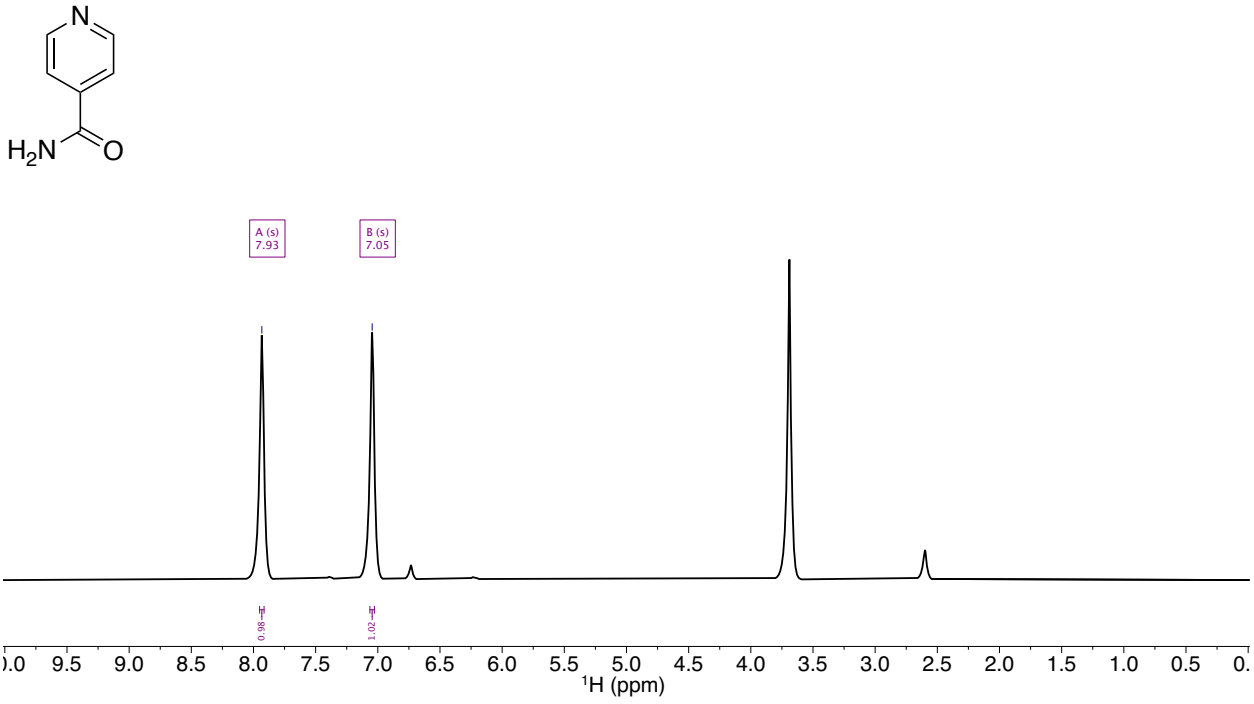


Figure S9. ^{1}H NMR spectrum of isonicotinamide **9** in $CDCl_3$:DMSO-d_6 = 1:1 at 25 °C.

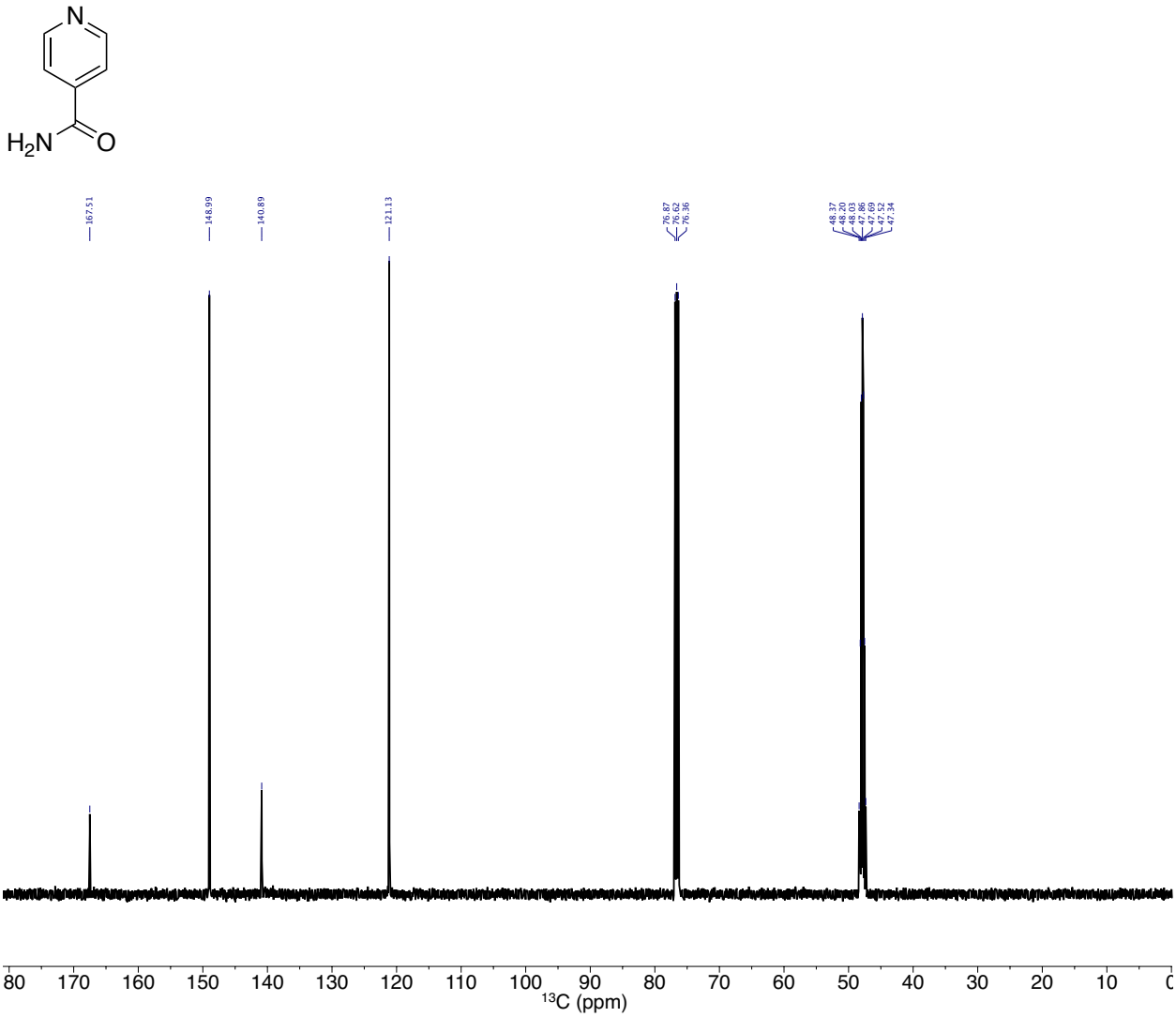
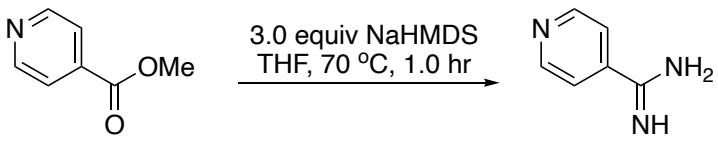


Figure S10. ^{13}C NMR spectrum of isonicotinamide **9** in $CDCl_3$:DMSO-d_6 = 1:1 at 25 °C.

Synthesis of isonicotinimidamide 10



Solid sodium hexamethyldisilazide (NaHMDS, 330 mg, 1.8 mmol) was dissolved in 3.0 mL of THF at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar, containing 42 mg of methyl isonicotinate **8** (0.30 mmol). The reaction was stirred at 70 °C for 1.0 hr. Rotavap THF. DI water (1.0 mL) was then added. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 1 hr. Saturated NaOH solution was then added until pH = 12. Mixture was partitioned between water (1.0 mL) and chloroform (4.0 mL). The aqueous layer was separated and extracted further with three 4.0 mL portions of chloroform. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated to afford product 34.8 mg (96%) of product isonicotinimidamide **10** as an off-white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.4 (m, 2H), 7.3 (m, 2H), 5.7 (s, 3H).

$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 162.7, 150.2, 143.6, 120.6.

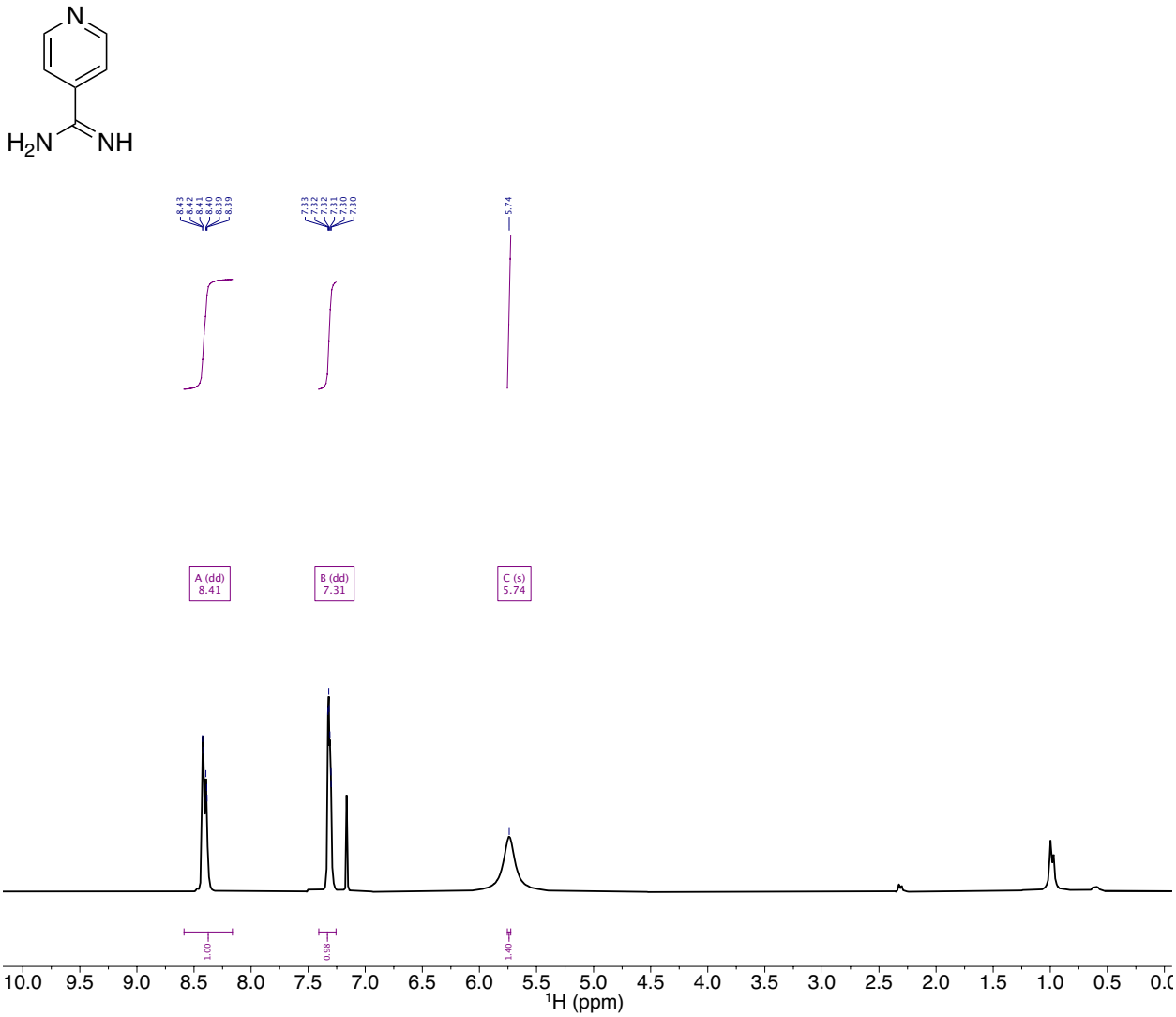


Figure S11. ^{1}H NMR spectrum of isonicotinimidamide **10** in $CDCl_3$:DMSO-d_6 = 7:1 at 25 °C.

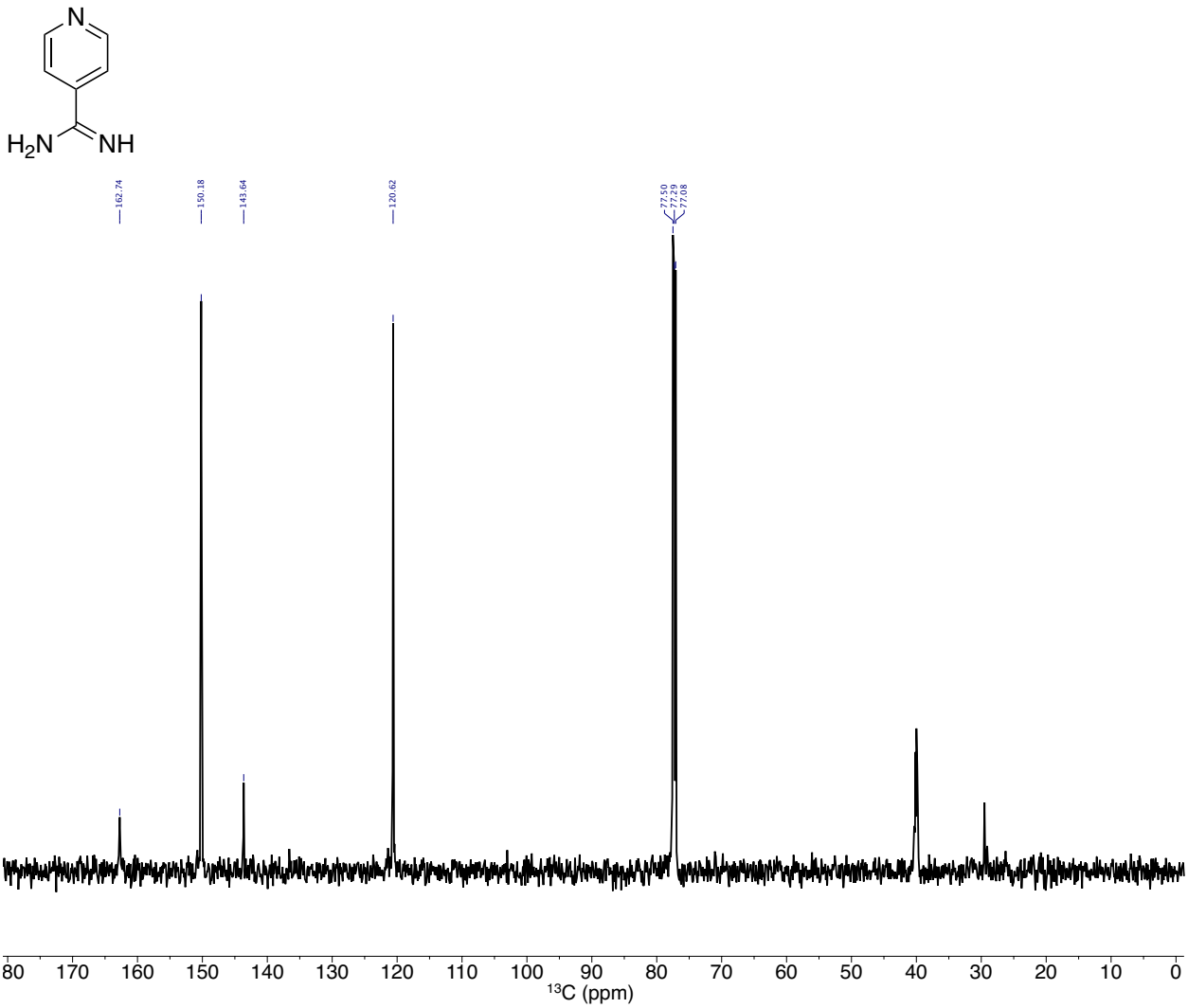
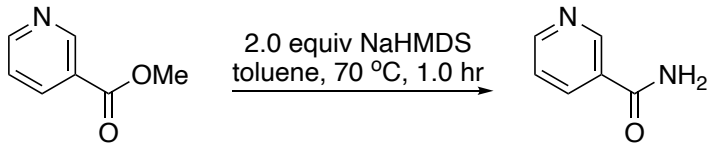


Figure S12. ^{13}C NMR spectrum of isonicotinimidamide **10** in $CDCl_3$:DMSO-d_6 = 7:1 at 25 °C.

Synthesis of nicotinamide 12



Solid sodium hexamethyldisilazide (NaHMDS, 165 mg, 0.9 mmol) was dissolved in 2.0 mL of toluene at 25 °C. 1.5 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar, containing 42 mg of methyl nicotinate **11** (0.30 mmol). The reaction was stirred at 70 °C for 1.0 hr. DI water (1.0 mL) was added, and the resulting biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (80% ethyl acetate in hexanes) afforded 27.8 mg (76%) of product nicotinamide **12** as a off white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.5 (m, 1H), 8.1 (m, 1H), 7.6 (m, 1H), 7.5 (s, 1H), 6.8 (d, *J* = 7.9 Hz, 1H), 6.6 (s, 1H).

$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 166.1, 150.7, 147.9, 134.2, 128.6, 121.9, 121.9.

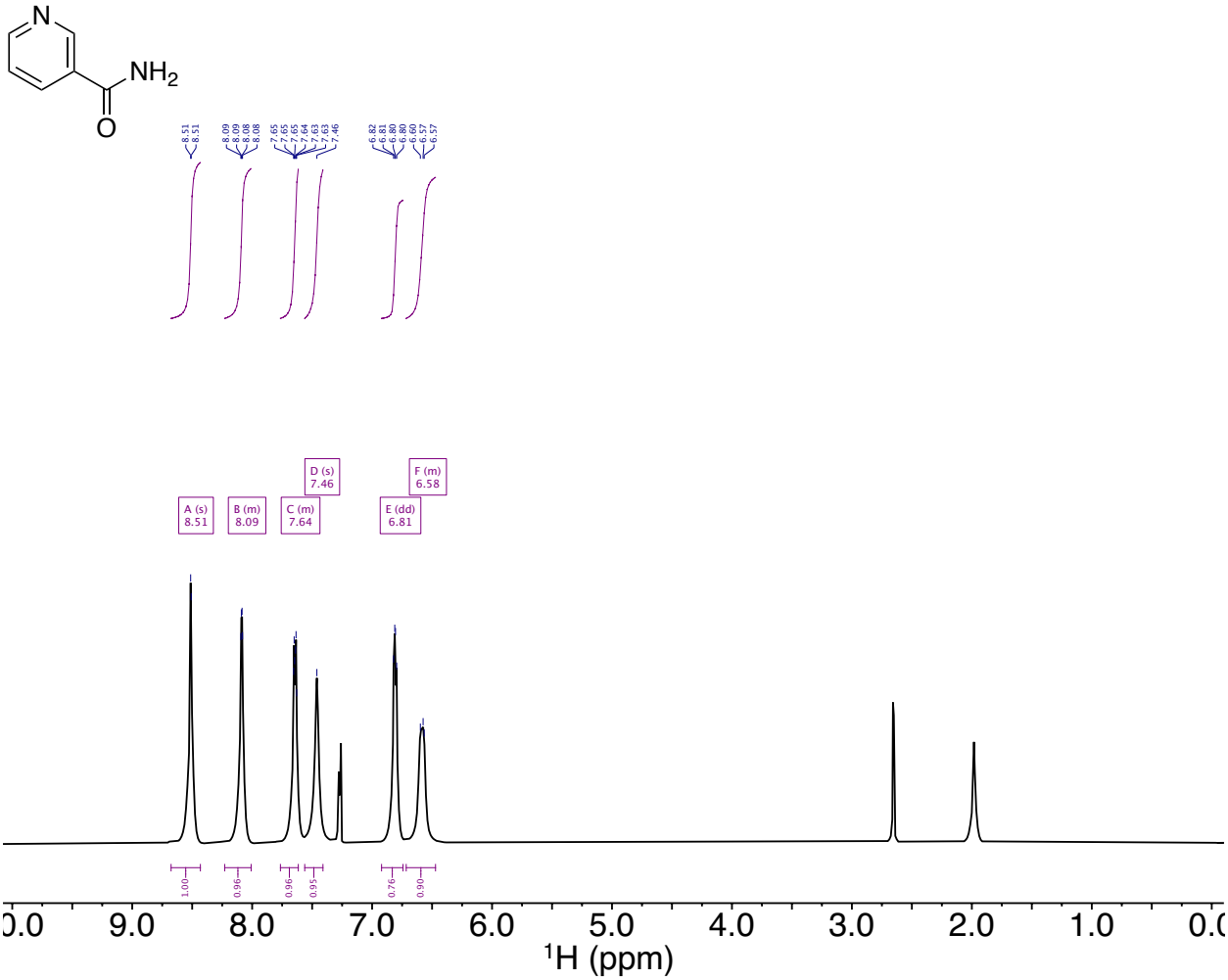


Figure S13. ^{1}H NMR spectrum of nicotinamide **12** in $CDCl_3$:DMSO-d_6 = 1:1 at 25 °C.

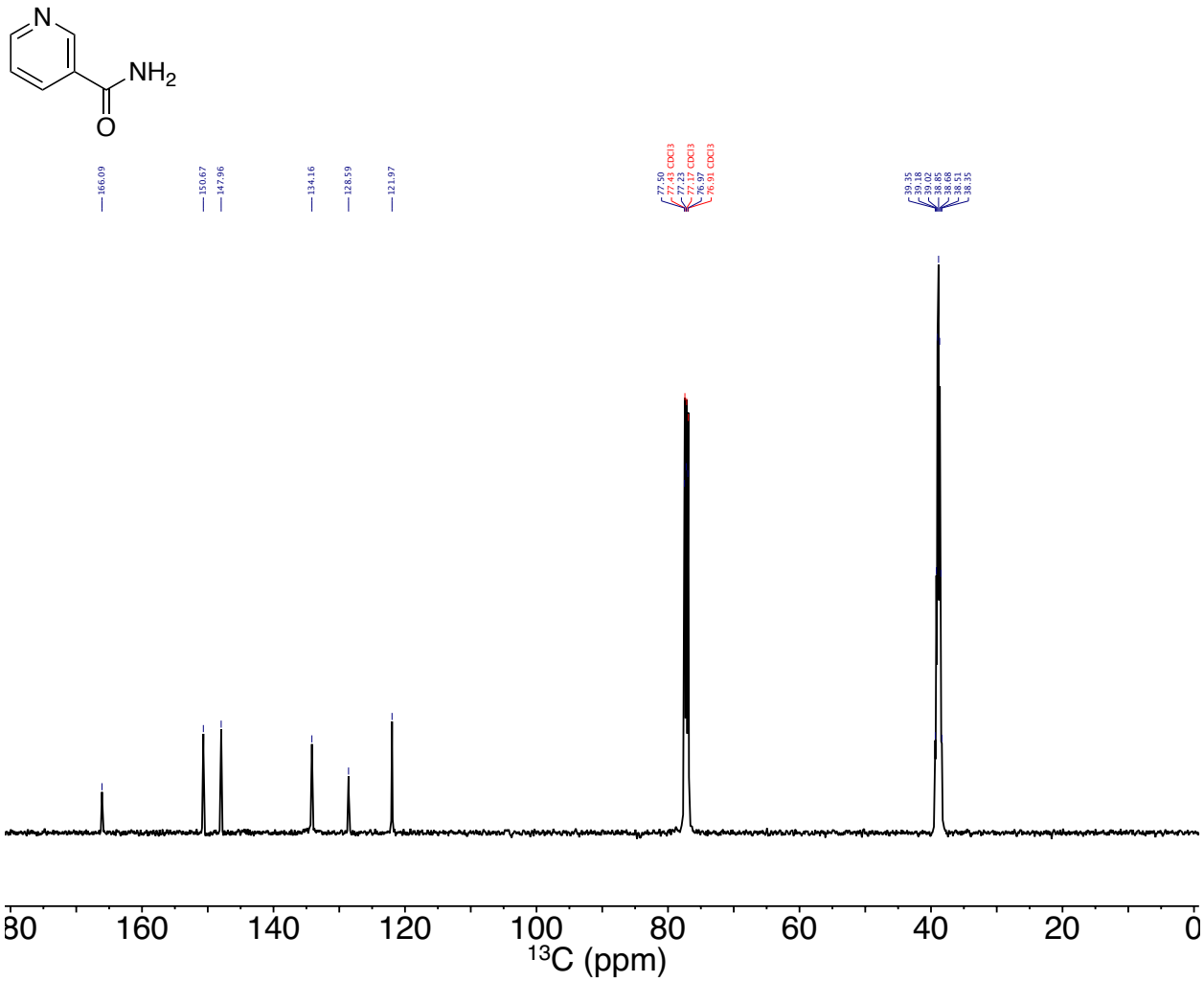
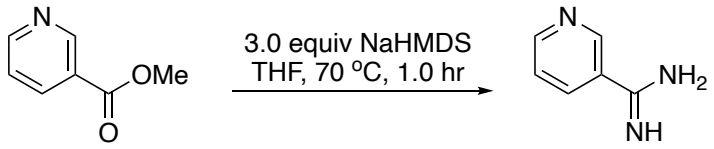


Figure S14. ^{13}C NMR spectrum of nicotinamide **12** in $CDCl_3$:DMSO-d_6 = 1:1 at 25 °C.

Synthesis of nicotinimidamide 13



Solid sodium hexamethyldisilazide (NaHMDS, 330 mg, 1.8 mmol) was dissolved in 3.0 mL of THF at 25 °C. 1.5 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar, containing 42 mg of methyl nicotinate **11** (0.30 mmol). The reaction was stirred at 70 °C for 1.0 hr. Rotavap THF. DI water (1.0 mL) was then added. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 1 hr. Saturated NaOH solution was then added until pH = 12. Mixture was partitioned between water (1.0 mL) and chloroform (4.0 mL). The aqueous layer was separated and extracted further with three 4.0 mL portions of chloroform. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated to afford product 34.4 mg (95%) of product nicotinimidamide **13** as a red oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.8 (d, *J* = 2.4 Hz, 1H), 8.7 (dt, *J* = 4.9, 1.5 Hz, 1H), 7.9 (dt, *J* = 8.1, 2.1 Hz, 1H), 7.3 (dd, *J* = 7.9, 4.9 Hz, 1H), 5.7 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 163.2, 151.4, 147.4, 133.8, 132.2, 123.5.

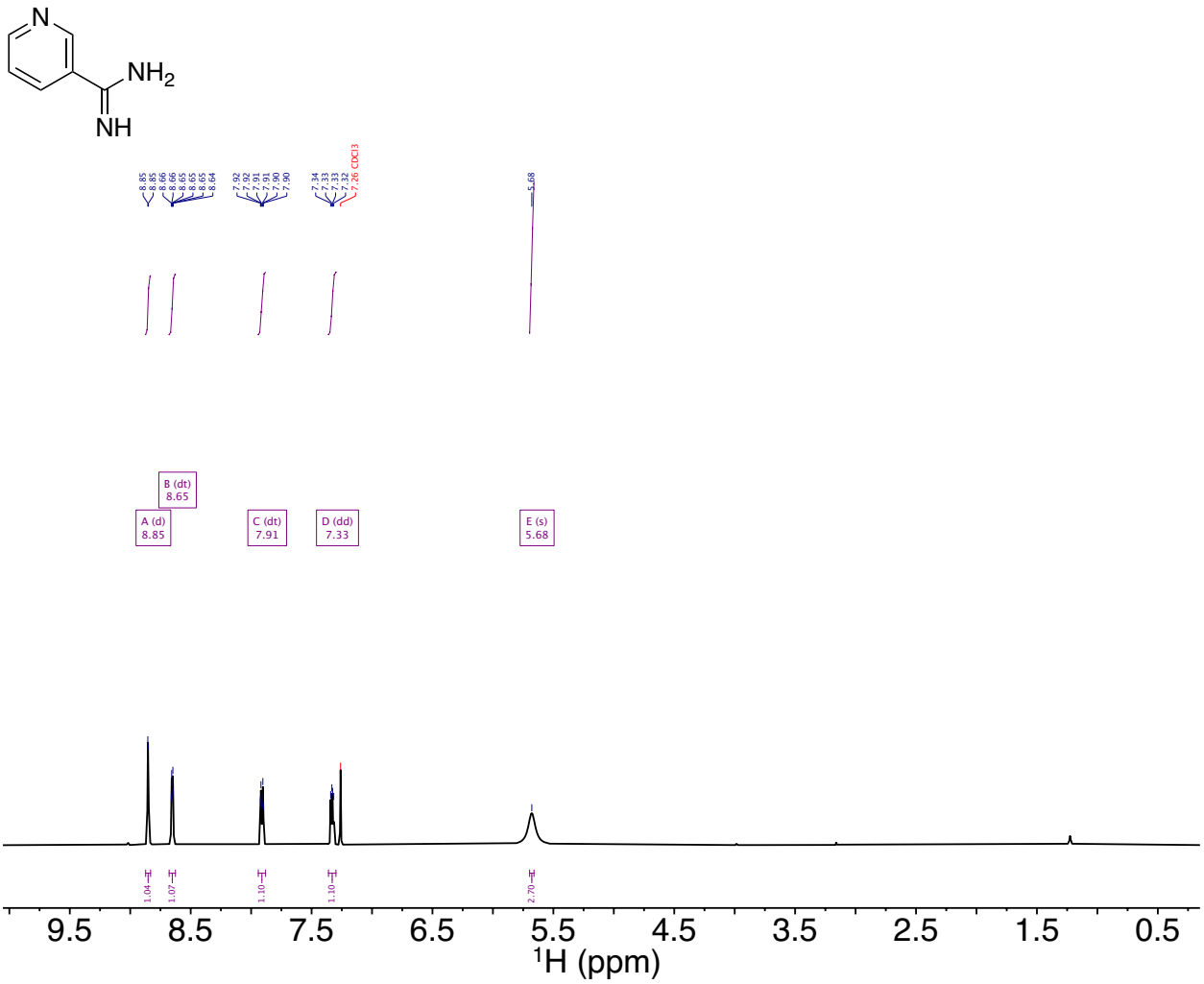


Figure S15. ^{1}H NMR spectrum of nicotinimidamide **13** in $CDCl_3$ at 25 °C.

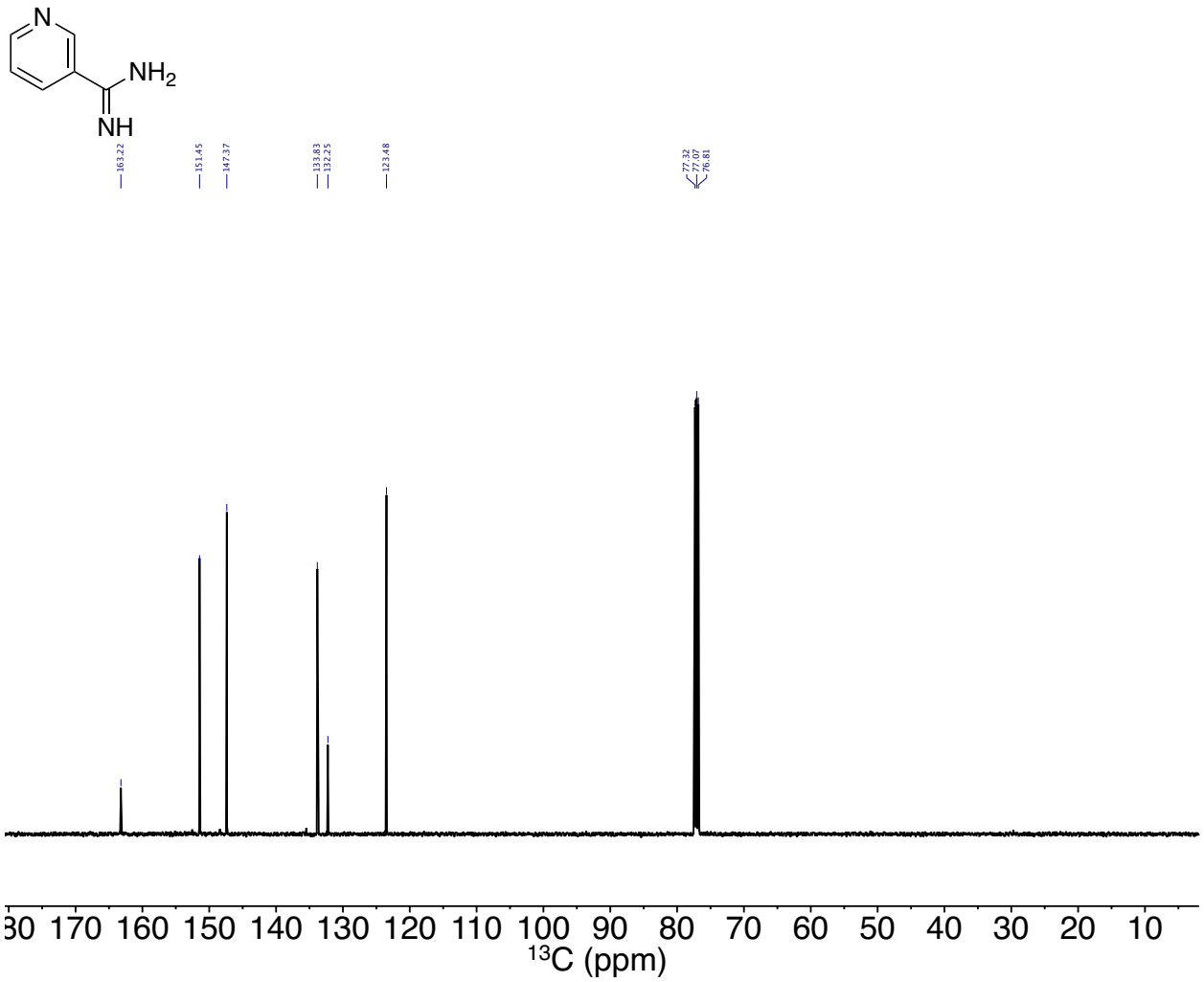
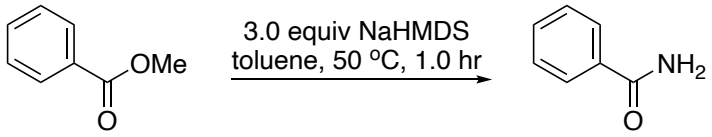


Figure S16. ^{13}C NMR spectrum of nicotinimidamide **13** in $CDCl_3$ at 25 °C.

Synthesis of benzamide 15



Solid sodium hexamethyldisilazide (NaHMDS, 110 mg, 0.6 mmol) was dissolved in 2.0 mL of toluene at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 38 µL of methyl benzoate **14** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 50 °C for 1.0 hr. DI water (1.0 mL) was added, and the resulting biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (40% ethyl acetate in hexanes) afforded 28.3 mg (78%) of product benzamide **15** as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.8 (dt, J = 7.0, 1.4 Hz, 2H), 7.5 (m, 1H), 7.4 (dd, J = 8.5, 7.0 Hz, 2H), 6.2 (s, 2H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 169.6, 133.4, 132.0, 128.6, 127.4.

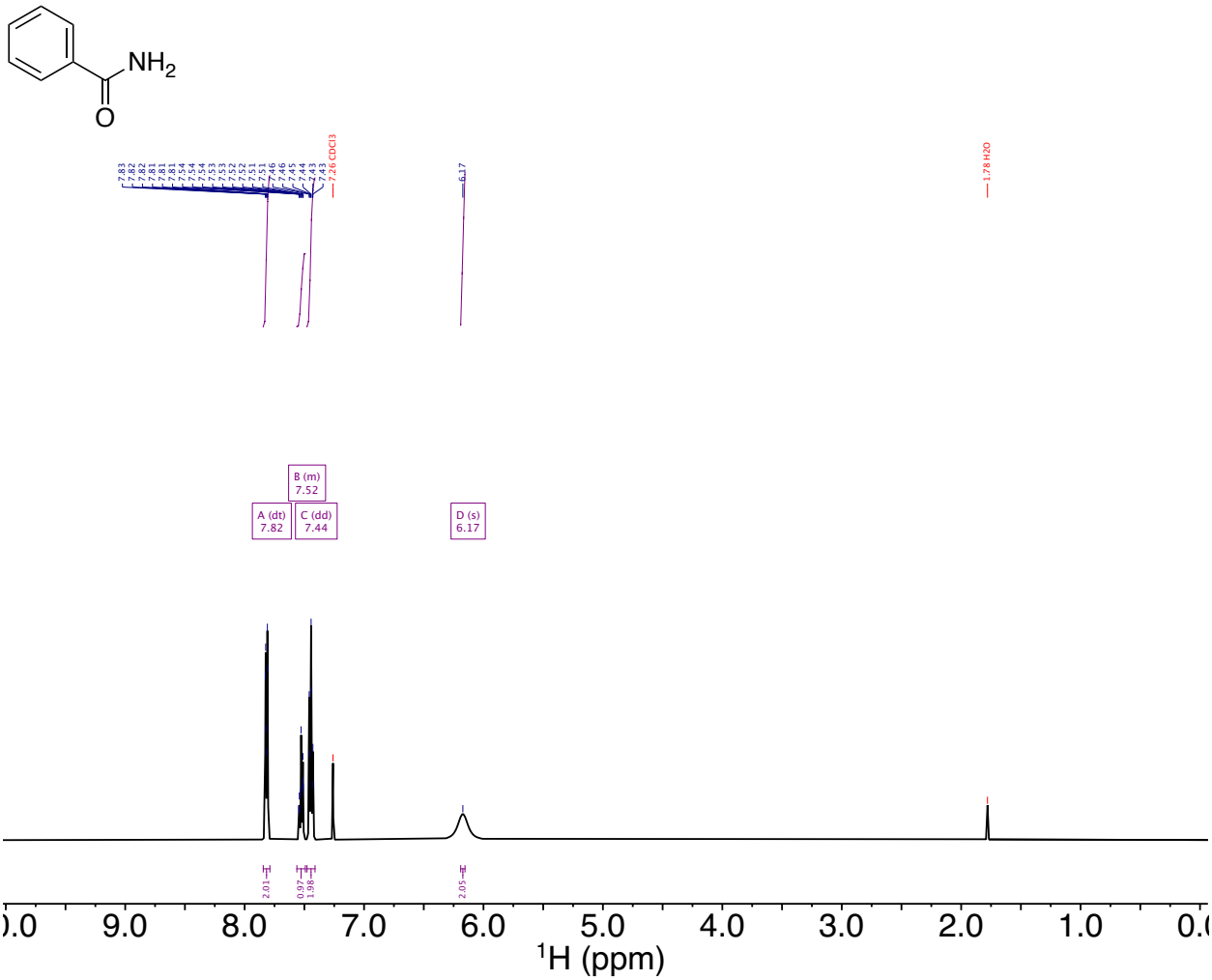


Figure S17. ^{1}H NMR spectrum of benzamide **15** in $CDCl_3$ at 25 °C.

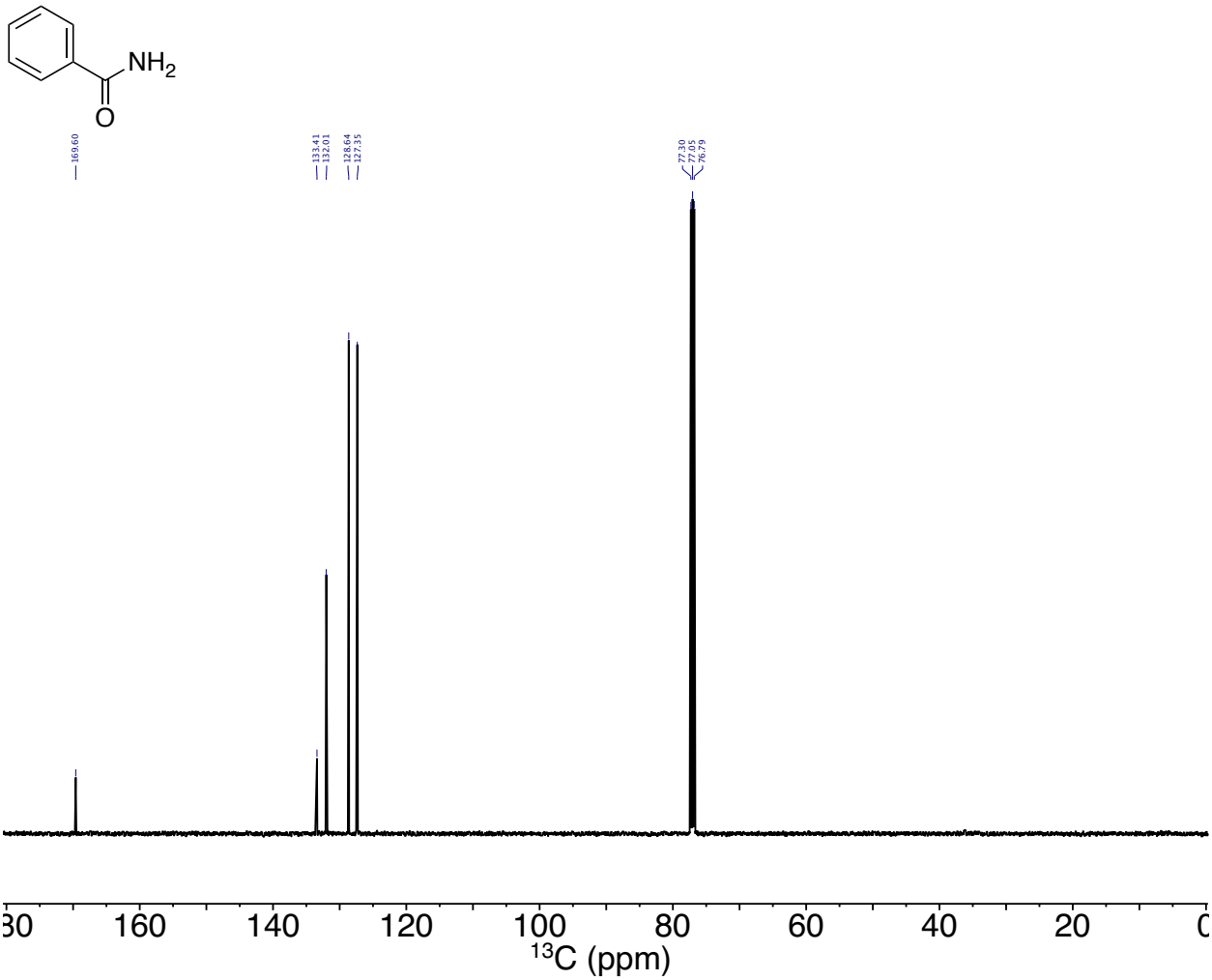
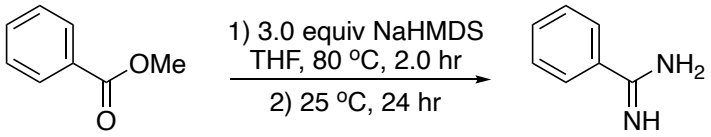


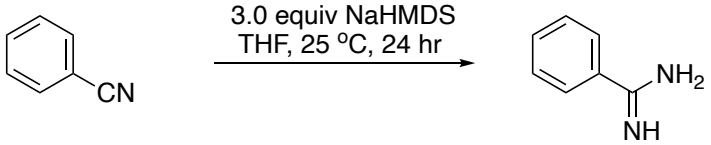
Figure S18. ^{13}C NMR spectrum of benzamide **15** in $CDCl_3$ at 25 °C.

Synthesis of benzimidamide 16 (a)



Solid sodium hexamethyldisilazide (NaHMDS, 330 mg, 1.8 mmol) was dissolved in 3.0 mL of THF at 25 °C. 1.5 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 38 µL of methyl benzoate **14** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 80 °C for 2.0 hr, then left at 25 °C for 24 hr. Rotavap THF. DI water (1.0 mL) was then added. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 1 hr. Saturated NaOH solution was then added until pH = 12. Mixture was partitioned between water (1.0 mL) and chloroform (4.0 mL). The aqueous layer was separated and extracted further with three 4.0 mL portions of chloroform. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated to afford product 34.4 mg (92%) of product benzimidamide **16** as a yellow solid.

Synthesis of benzimidamide 16 (b)



Solid sodium hexamethyldisilazide (NaHMDS, 330 mg, 1.8 mmol) was dissolved in 3.0 mL of THF at 25 °C. 1.5 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 31 µL of benzonitrile **17** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 25 °C for 24 hr. Rotavap THF. DI water (1.0 mL) was then added. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 1 hr. Saturated NaOH solution was then added until pH = 12. Mixture was partitioned between water (1.0 mL) and chloroform (4.0 mL). The aqueous layer was separated and extracted further with three 4.0 mL portions of chloroform. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated to afford product 34.2 mg (95%) of product benzimidamide **16** as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.6 (m 2H), 7.5 (m, 1H), 7.4 (qd, *J* = 7.8, 3.6 Hz, 3H), 5.6 (s, 3H).

$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 166.1, 136.5, 130.5, 128.8, 126.0.

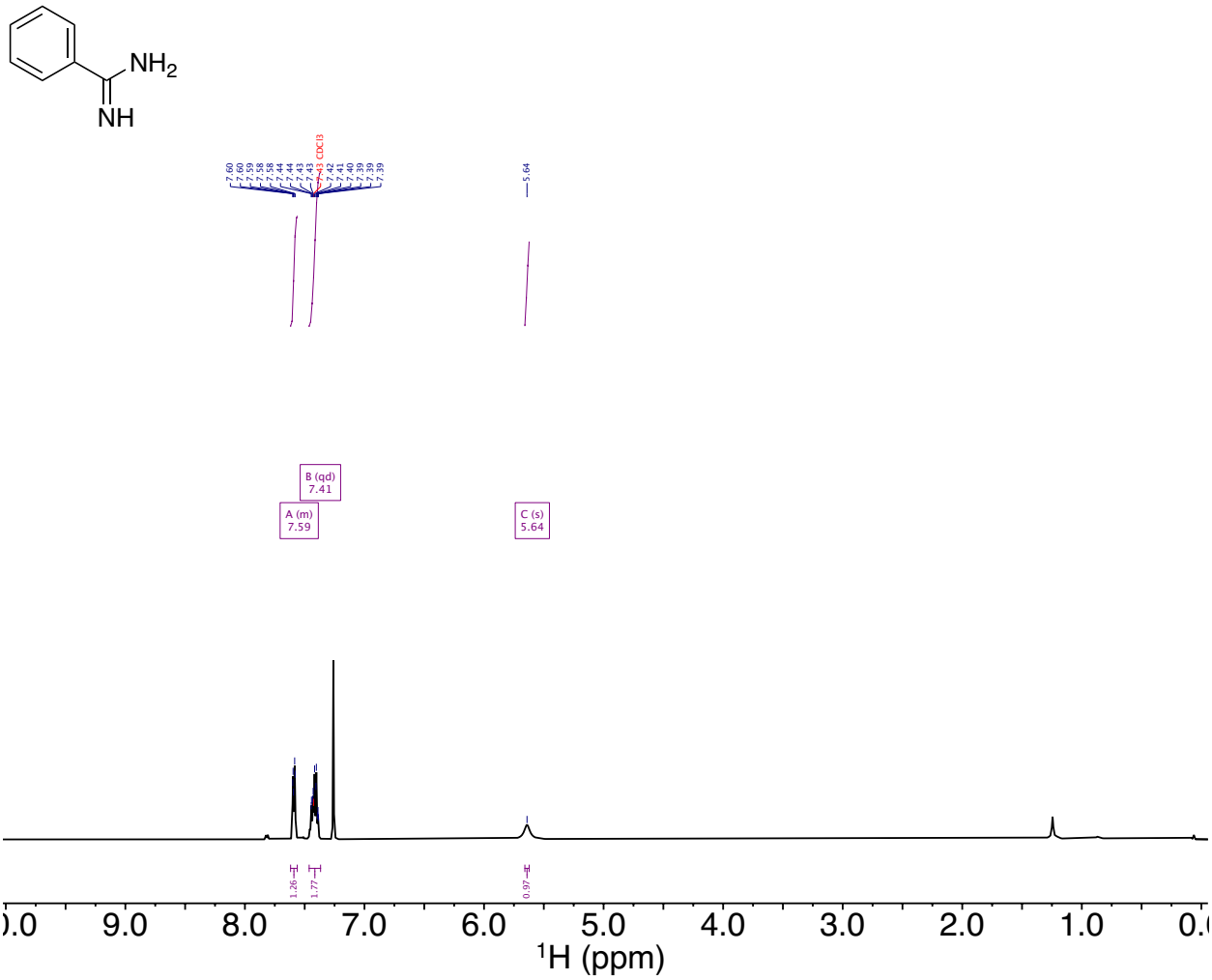


Figure S19. ^{1}H NMR spectrum of benzimidamide **16** in $CDCl_3$ at 25 °C.

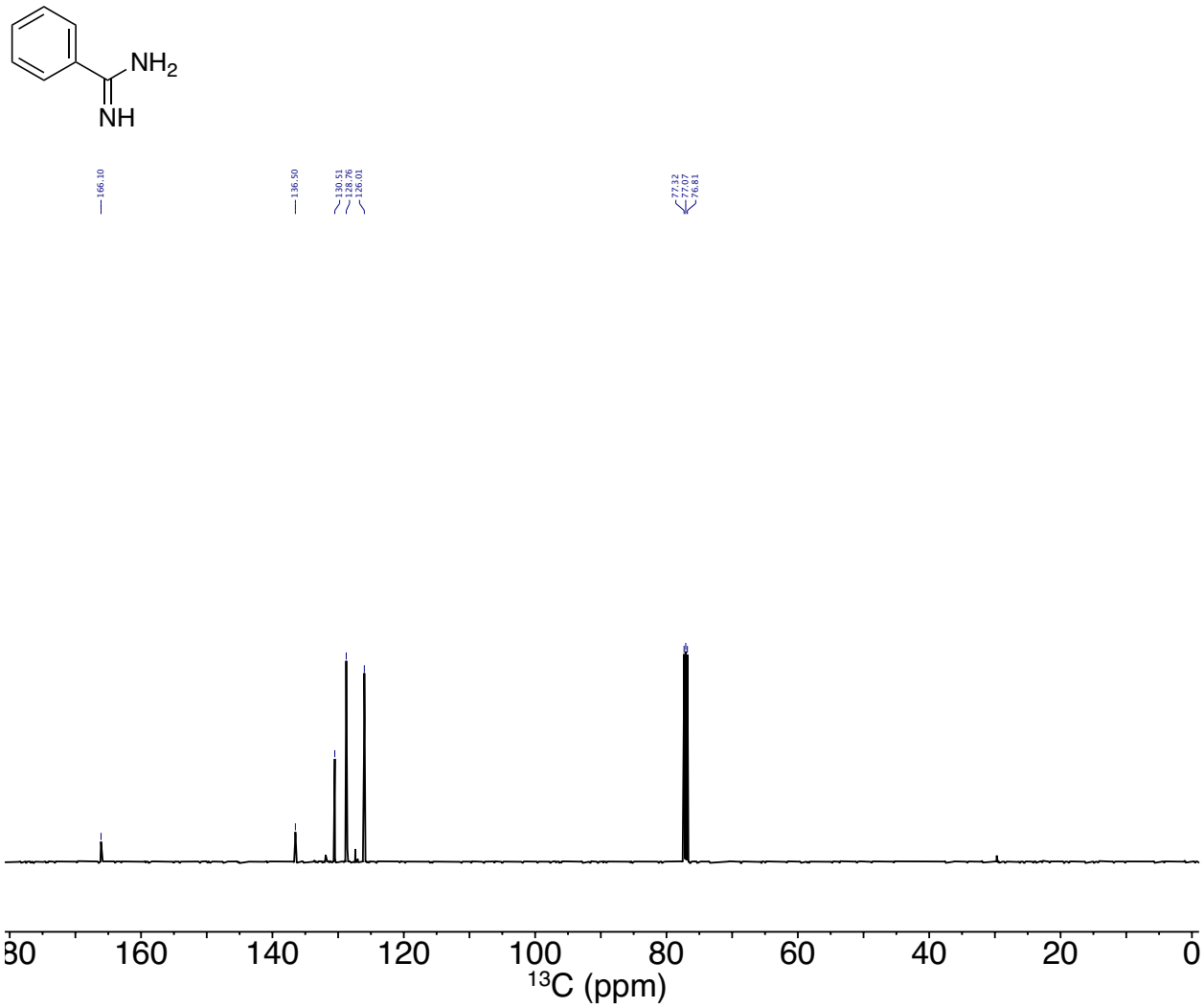
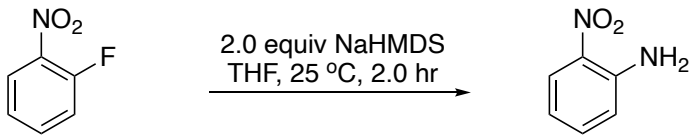


Figure S20. ^{13}C NMR spectrum of benzimidamide **16** in $CDCl_3$ at 25 °C.

Synthesis of 2-nitroaniline 19



Solid sodium hexamethyldisilazide (NaHMDS, 110 mg, 0.6 mmol) was dissolved in 2.0 mL of toluene at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 36 µL of 2-fluoronitrobenzene **18** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 25 °C for 2.0 hr. DI water (1.0 mL) was added, and the resulting biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (10% ethyl acetate in hexanes) afforded 35.2 mg (85%) of product 2-nitroaniline **19** as a yellow oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.1 (dd, J = 8.7, 1.5 Hz, 1H), 7.4 (ddd, J = 8.4, 7.0, 1.5 Hz, 1H), 6.8 (dd, J = 8.4, 1.3 Hz, 1H), 6.7 (ddd, J = 8.4, 7.0, 1.3 Hz, 1H), 6.1 (s, 2H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 144.6, 135.6, 132.3, 126.2, 118.7, 117.0.

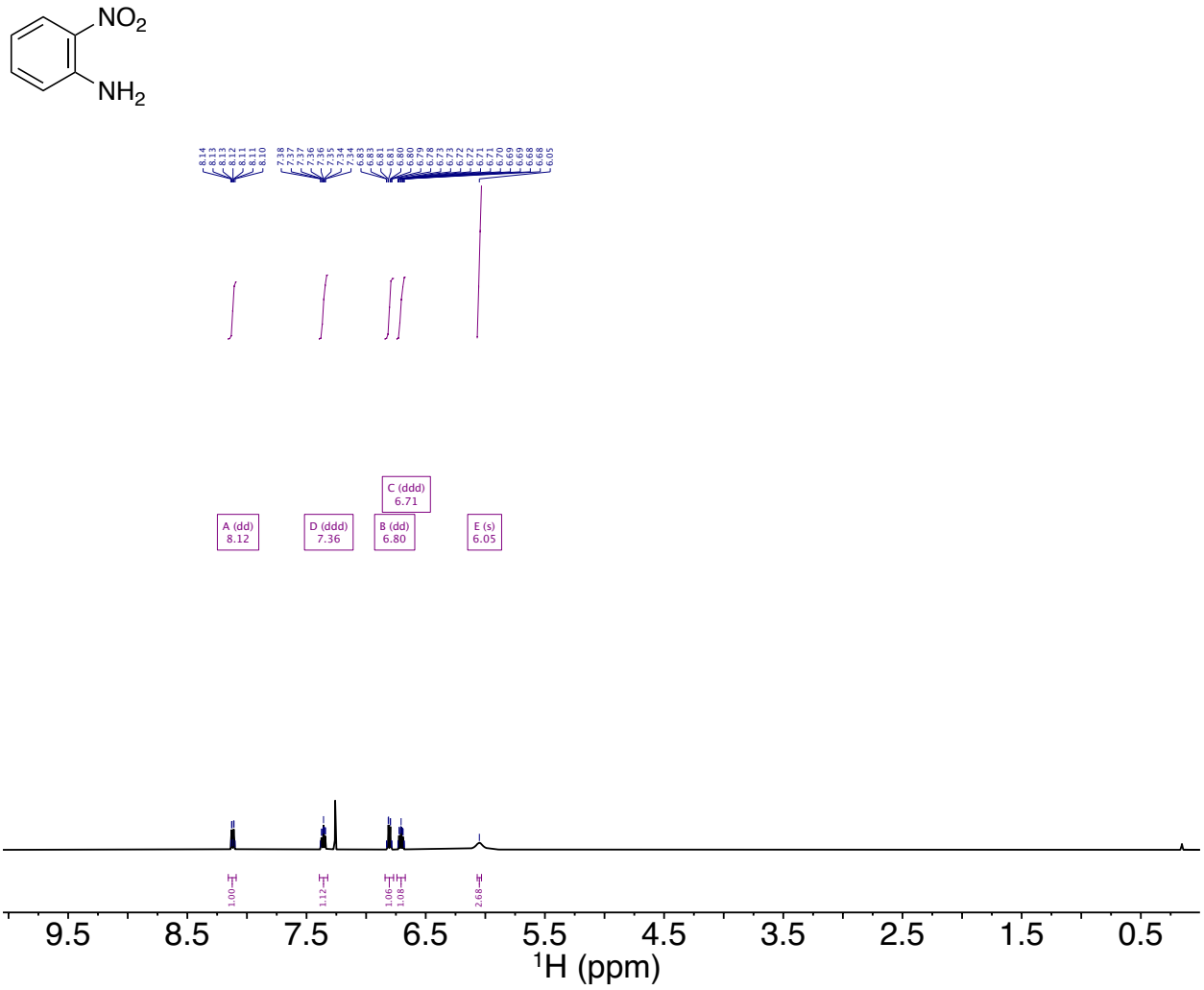


Figure S21. ^{1}H NMR spectrum of 2-nitroaniline **19** in $CDCl_3$ at 25 °C.

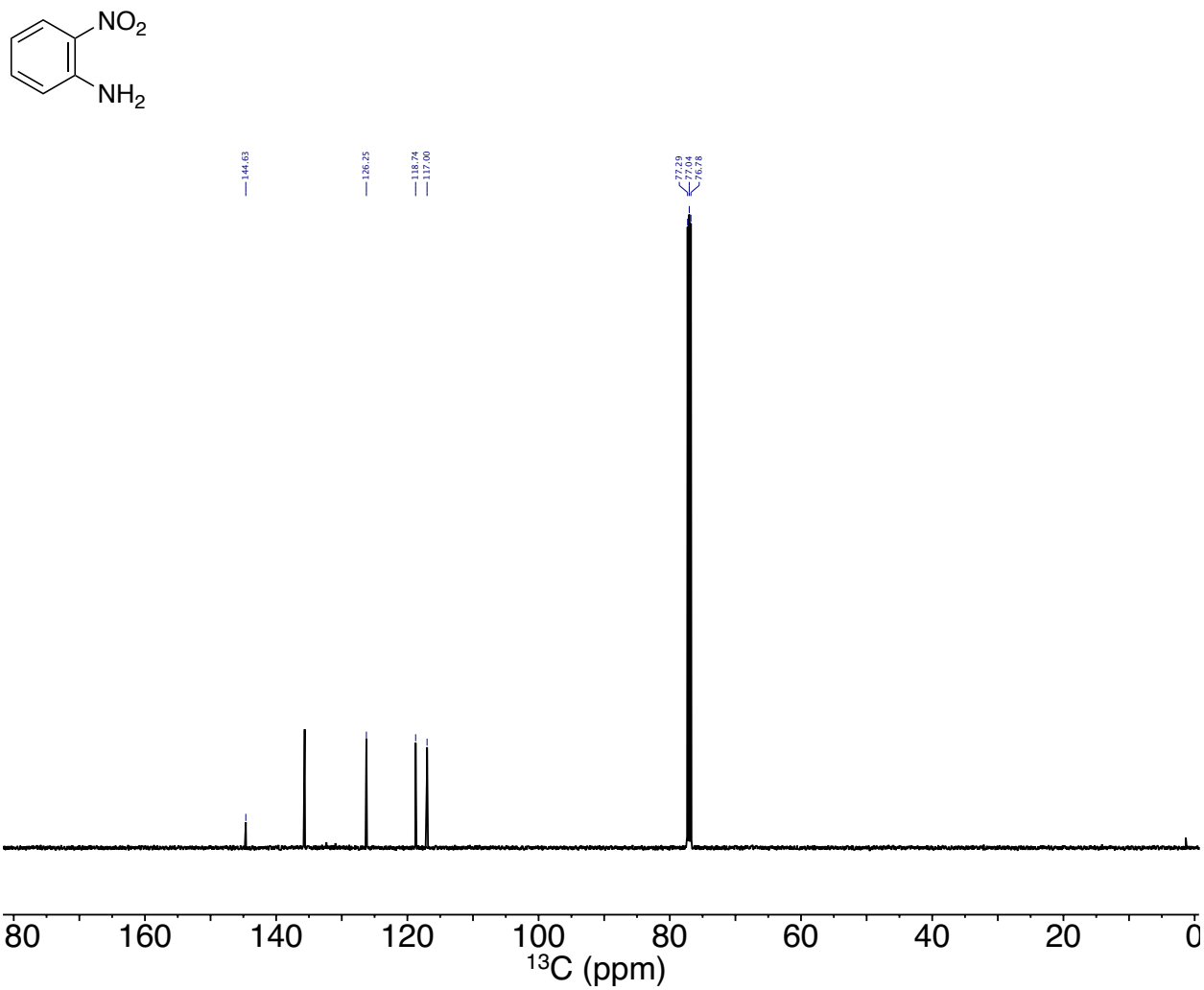
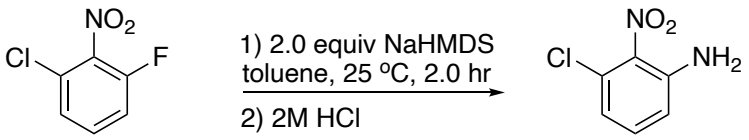


Figure S22. ^{13}C NMR spectrum of 2-nitroaniline **19** in $CDCl_3$ at 25 °C.

Synthesis of 3-chloro-2-nitroaniline 21



Solid sodium hexamethyldisilazide (NaHMDS, 110 mg, 0.6 mmol) was dissolved in 2.0 mL of toleune at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 36 µL of 1-chloro-3-fluoro-2-nitrobenzene **20** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 25 °C for 2.0 hr. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 24 hr. Saturated NaOH solution was then added until pH = 12. Biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (10% ethyl acetate in hexanes) afforded 39.8 mg (77%) of product 3-chloro-2-nitroaniline **21** as a “red-brown” solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.2 (t, *J* = 8.1 Hz, 1H), 6.8 (d, *J* = 7.9 Hz, 1H), 6.7 (d, *J* = 8.4 Hz, 1H), 4.9 (s, 2H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 143.0, 135.2, 132.6, 128.3, 120.1, 116.6.

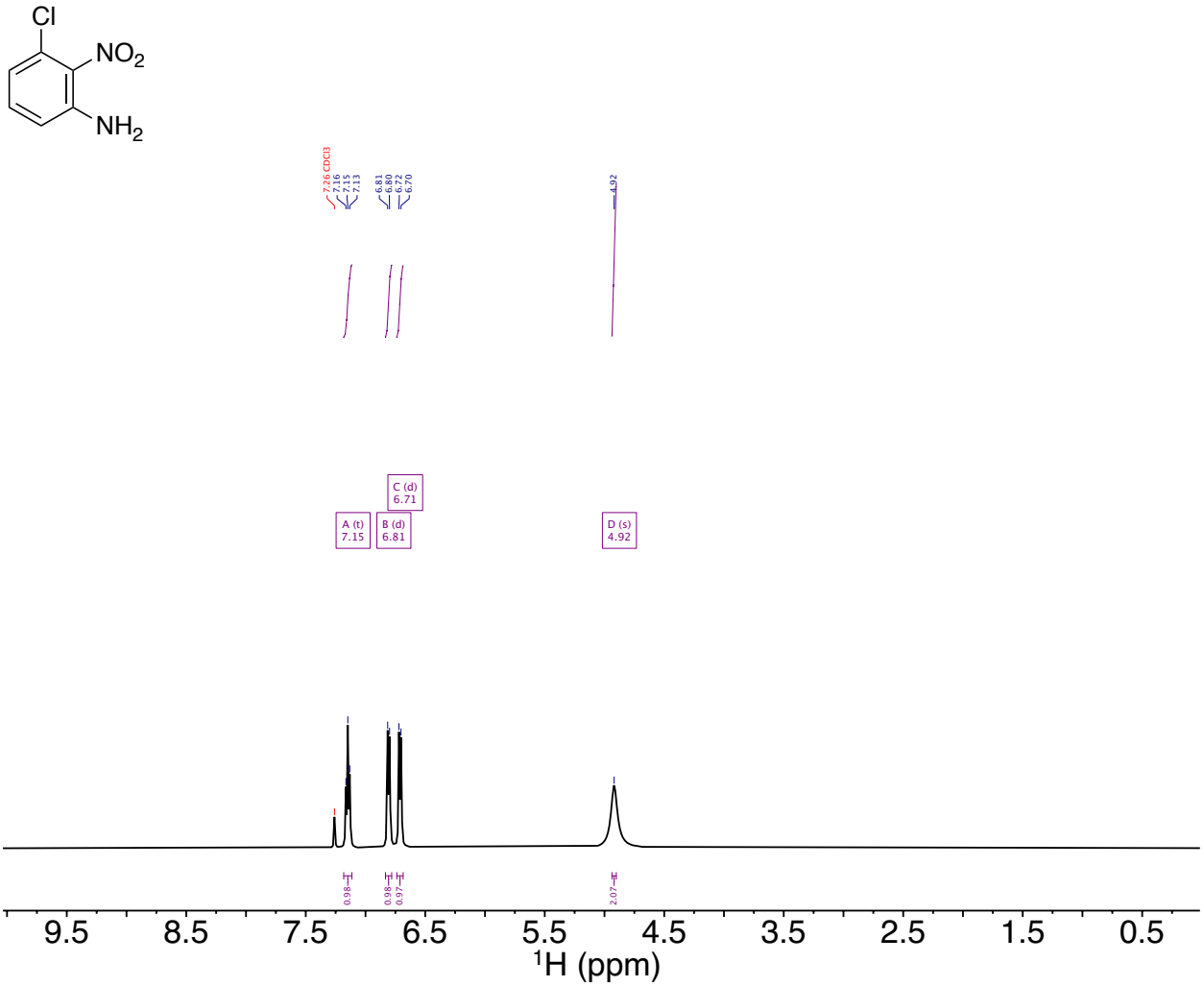


Figure S23. ^{1}H NMR spectrum of 3-chloro-2-nitroaniline **21** in $CDCl_3$ at 25 °C.

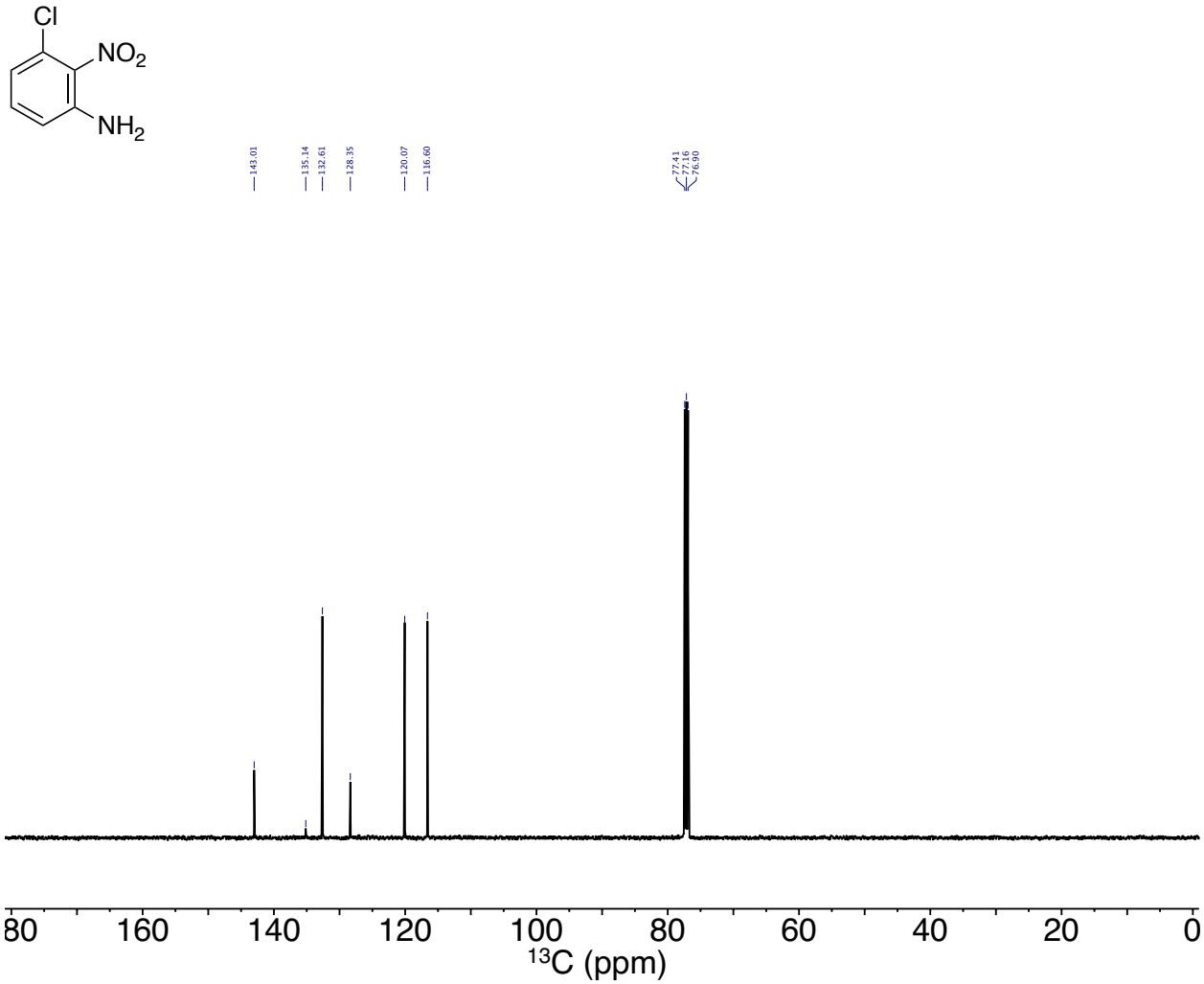
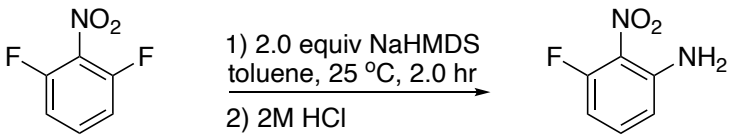


Figure S24. ^{13}C NMR spectrum of 3-chloro-2-nitroaniline **21** in $CDCl_3$ at 25 °C.

Synthesis of 3-fluoro-2-nitroaniline 23



Solid sodium hexamethyldisilazide (NaHMDS, 110 mg, 0.6 mmol) was dissolved in 2.0 mL of toleune at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 35 µL of 2,6-difluoronitrobenzene **22** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 25 °C for 2.0 hr. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 24 hr. Saturated NaOH solution was then added until pH = 12. Biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (10% ethyl acetate in hexanes) afforded 40.2 mg (85%) of product 3-fluoro-2-nitroaniline **23** as a brown solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.2 (td, *J* = 8.3, 5.4 Hz, 1H), 6.6 (d, *J* = 8.5, 1.5 Hz, 1H), 6.7 (ddd, *J* = 11.4, 8.1, 1.3 Hz, 1H), 5.7 (s, 2H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 158.5, 156.4, 145.1, 135.6, 134.3, 134.3, 124.9, 113.5, 113.5, 104.8, 104.6, 104.6.

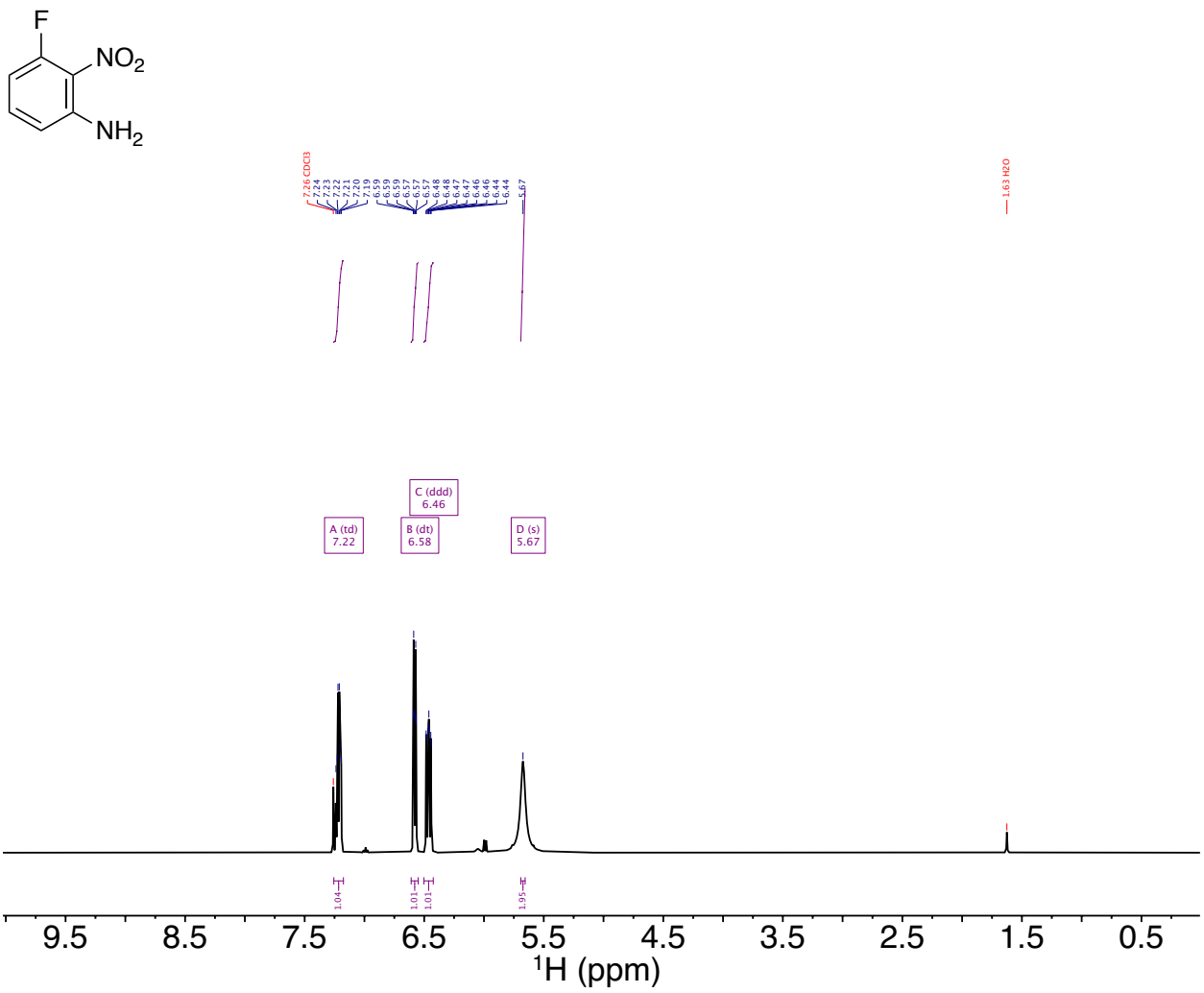


Figure S25. ^{1}H NMR spectrum of 3-fluoro-2-nitroaniline **23** in $CDCl_3$ at 25 °C.

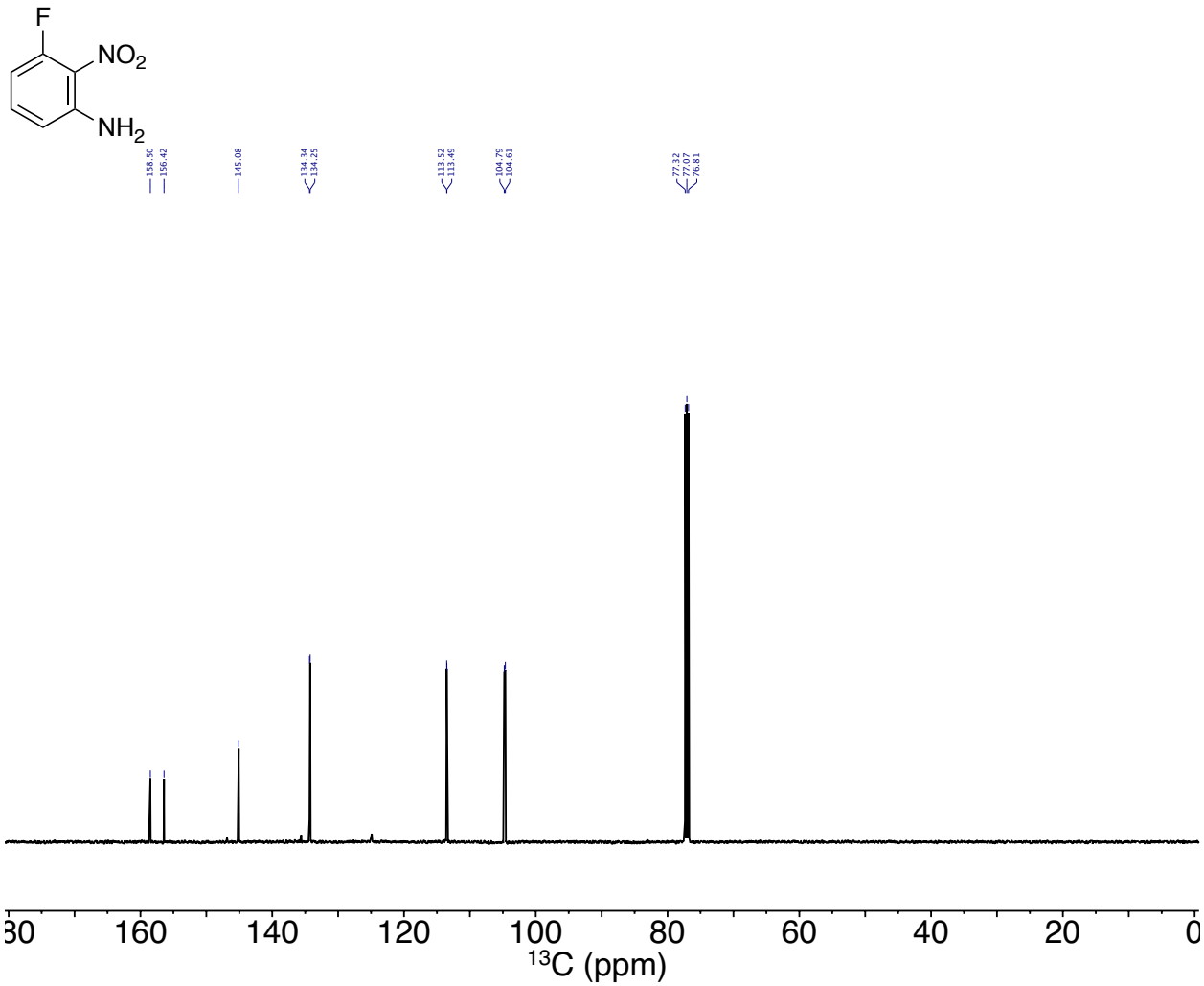
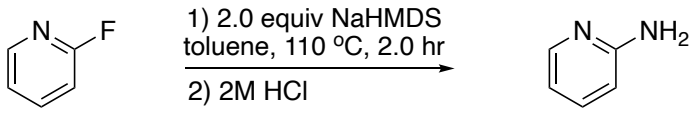


Figure S26. ^{13}C NMR spectrum of 3-fluoro-2-nitroaniline **23** in $CDCl_3$ at 25 °C.

Synthesis of pyridin-2-amine 25



Solid sodium hexamethyldisilazide (NaHMDS, 110 mg, 0.6 mmol) was dissolved in 2.0 mL of toleune at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 31 µL of 2-fluoropyridine **24** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 110 °C for 2.0 hr. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 24 hr. Saturated NaOH solution was then added until pH = 12. Biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (20% ethyl acetate in hexanes) afforded 15.6 mg (55%) of product pyridin-2-amine **25** as an off-white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.1 (d, J = 5.4, 2.0 Hz, 1H), 7.4 (ddd, J = 8.6, 7.1, 1.9 Hz, 1H), 6.6 (ddd, J = 7.2, 5.1, 1.0 Hz, 1H), 6.5 (m, 1H), 4.5 (s, 2H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 158.6, 148.2, 137.8, 114.4, 108.7.

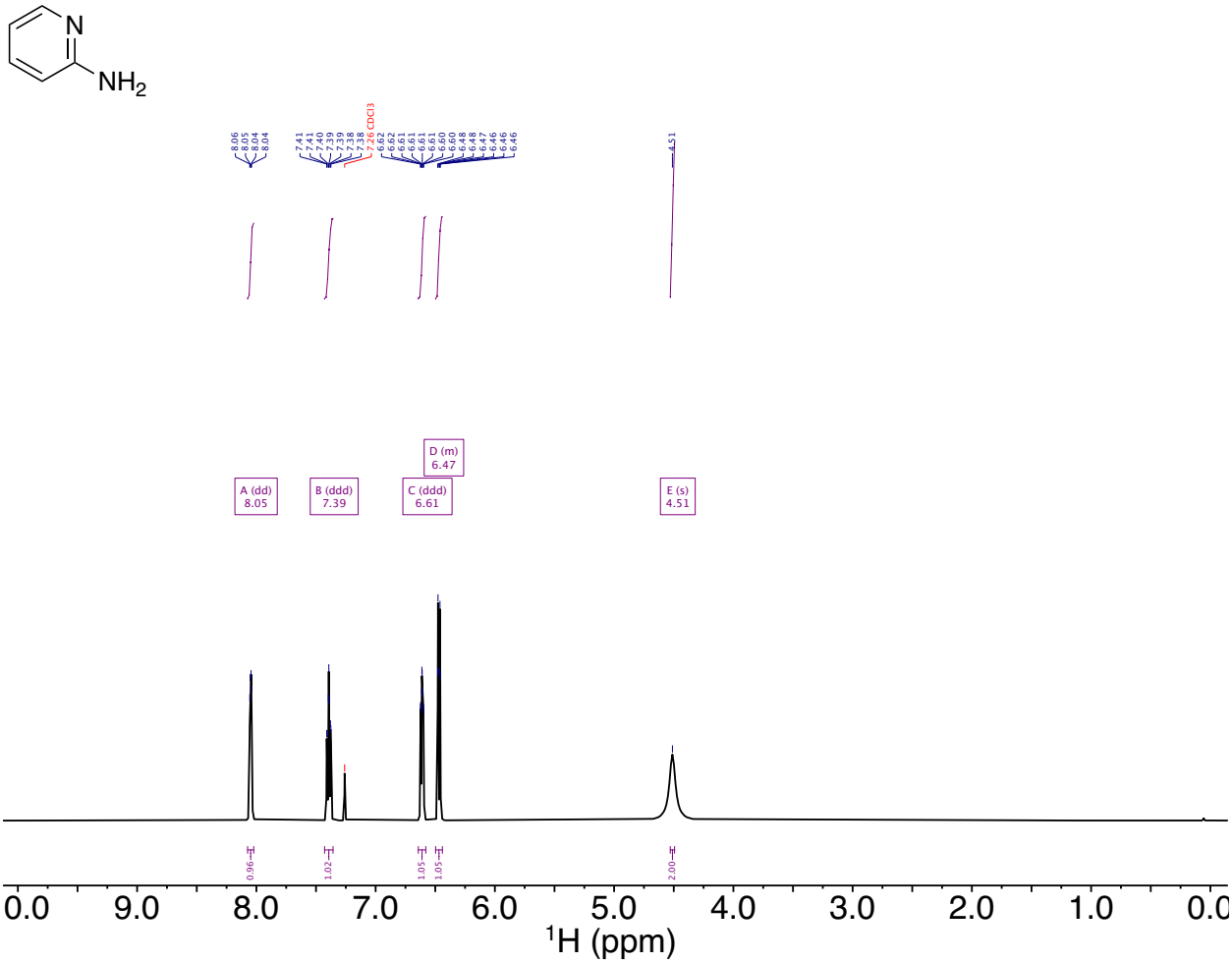


Figure S27. ^{1}H NMR spectrum of pyridin-2-amine **25** in $CDCl_3$ at 25 °C.

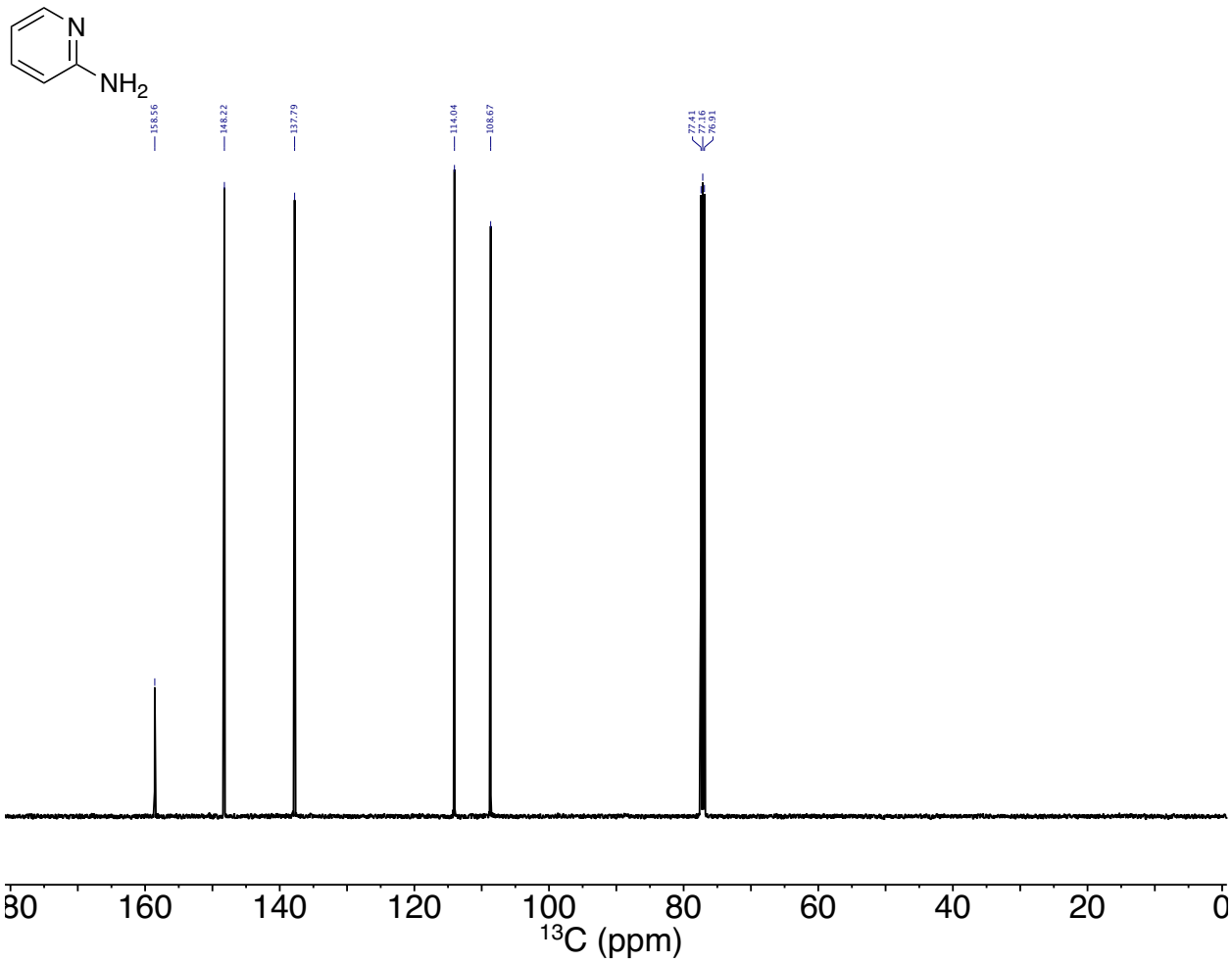
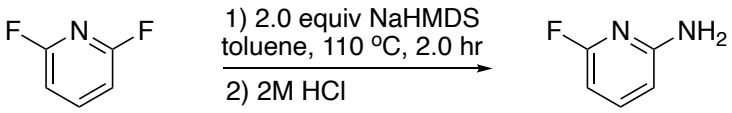


Figure S28. ^{13}C NMR spectrum of pyridin-2-amine **25** in $CDCl_3$ at 25 °C.

Synthesis of 6-fluoropyridin-2-amine 27



Solid sodium hexamethyldisilazide (NaHMDS, 110 mg, 0.6 mmol) was dissolved in 2.0 mL of toleune at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 28 µL of 2,6-difluoropyridine **26** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 110 °C for 2.0 hr. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 24 hr. Saturated NaOH solution was then added until pH = 12. Biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (20% ethyl acetate in hexanes) afforded 25.6 mg (76%) of product 6-fluoropyridin-2-amine **27** as an off-white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.5 (q, *J* = 8.0 Hz, 1H), 6.3 (dd, *J* = 7.9, 2.3 Hz, 1H), 6.2 (dd, *J* = 7.8, 2.2 Hz, 1H), 4.7 (s, 2H).

$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 164.2, 162.3, 157.9, 157.7, 142.2, 142.2, 104.6, 104.6, 97.1, 96.8.

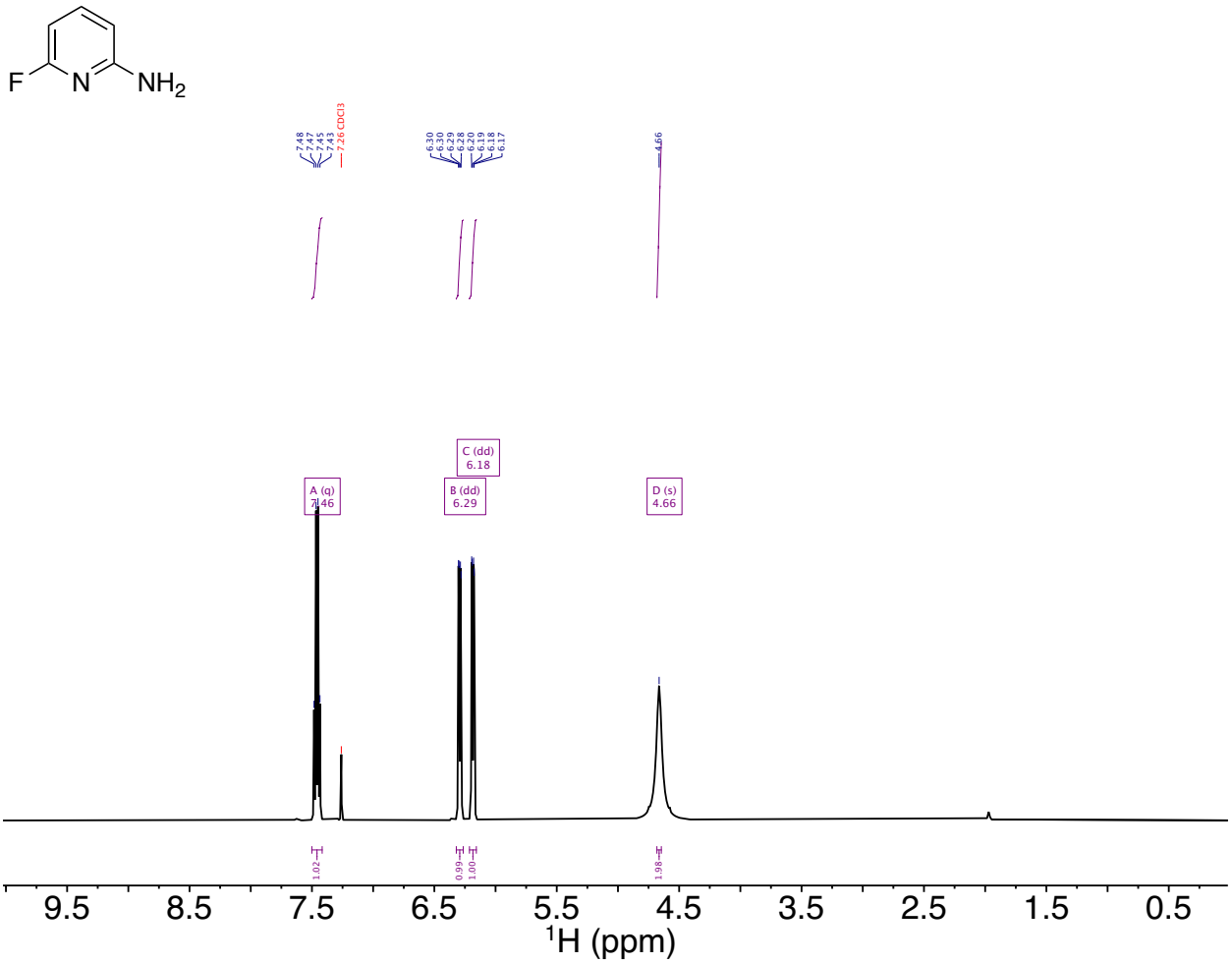


Figure S29. ^{1}H NMR spectrum of 6-fluoropyridin-2-amine **27** in $CDCl_3$ at 25 °C.

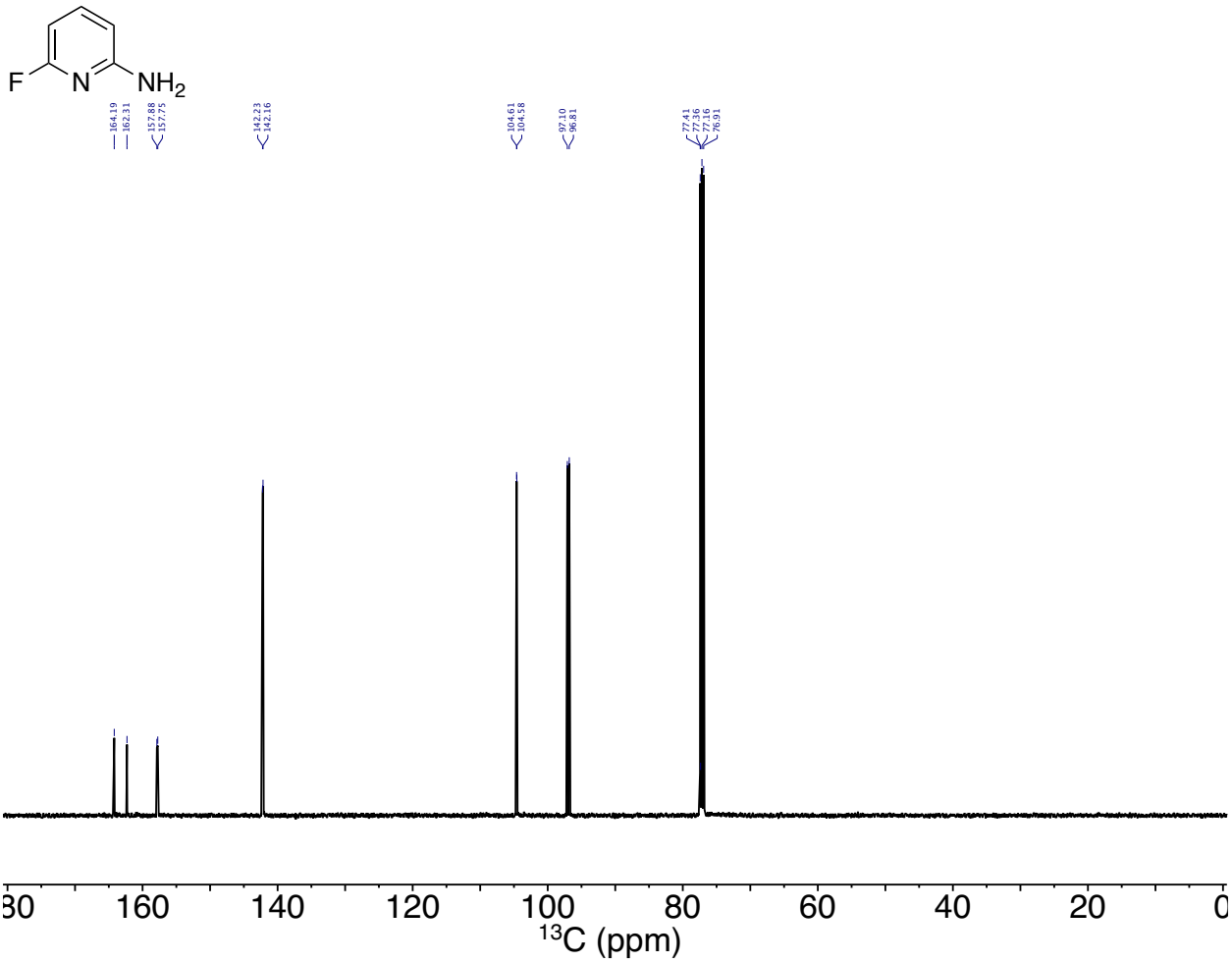
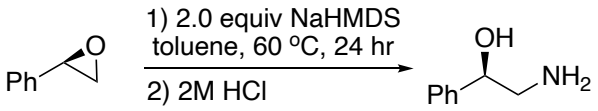


Figure S30. ^{13}C NMR spectrum of 6-fluoropyridin-2-amine **27** in $CDCl_3$ at 25 °C.

Synthesis of (*R*)-2-amino-1-phenylethan-1-ol 29



Solid sodium hexamethyldisilazide (NaHMDS, 110 mg, 0.6 mmol) was dissolved in 2.0 mL of toleune at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 35 µL of (*R*)-2-phenyloxirane **28** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 60 °C for 24 hr. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 24 hr. Saturated NaOH solution was then added until pH = 12. Biphasic mixture was partitioned between water (1.0 mL) and ethyl ether (2.0 mL). The aqueous layer was separated and extracted further with three 2.0 mL portions of ethyl ether. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (20% ethyl acetate in hexanes) afforded 35.4 mg (86%) of product (*R*)-2-amino-1-phenylethan-1-ol **29** as an off-white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.4 (m, 4H), 7.3 (m, 1H), 4.7 (dd, *J* = 7.9, 3.9 Hz, 1H), 3.0 (m, 1H), 2.8 (dd, *J* = 12.7, 7.8j Hz, 1H), 2.1 (s, 3H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 142.6, 128.6, 127.7, 126.0, 74.4, 49.3.

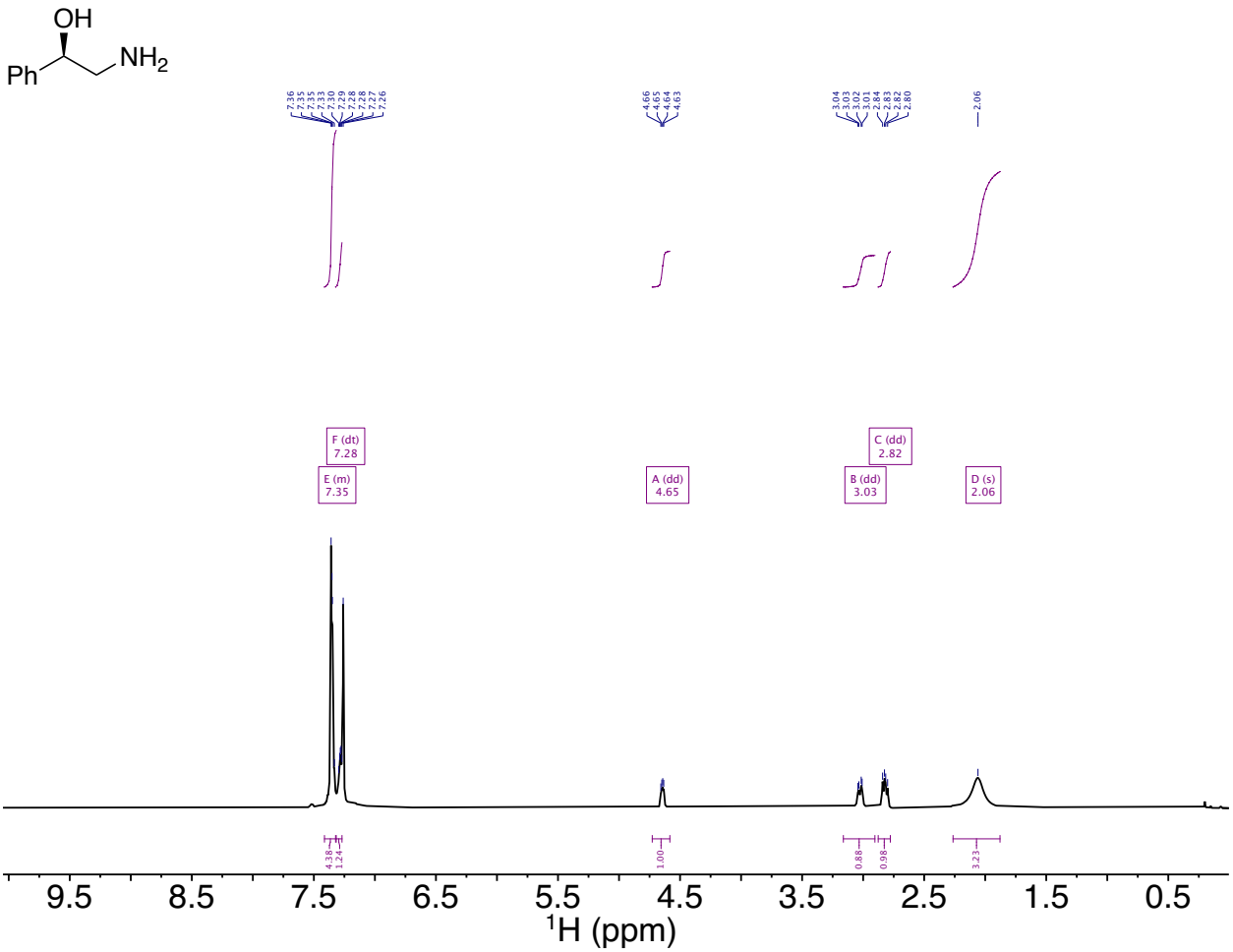


Figure S31. ^{1}H NMR spectrum of (*R*)-2-amino-1-phenylethan-1-ol **29** in $CDCl_3$ at 25 °C.

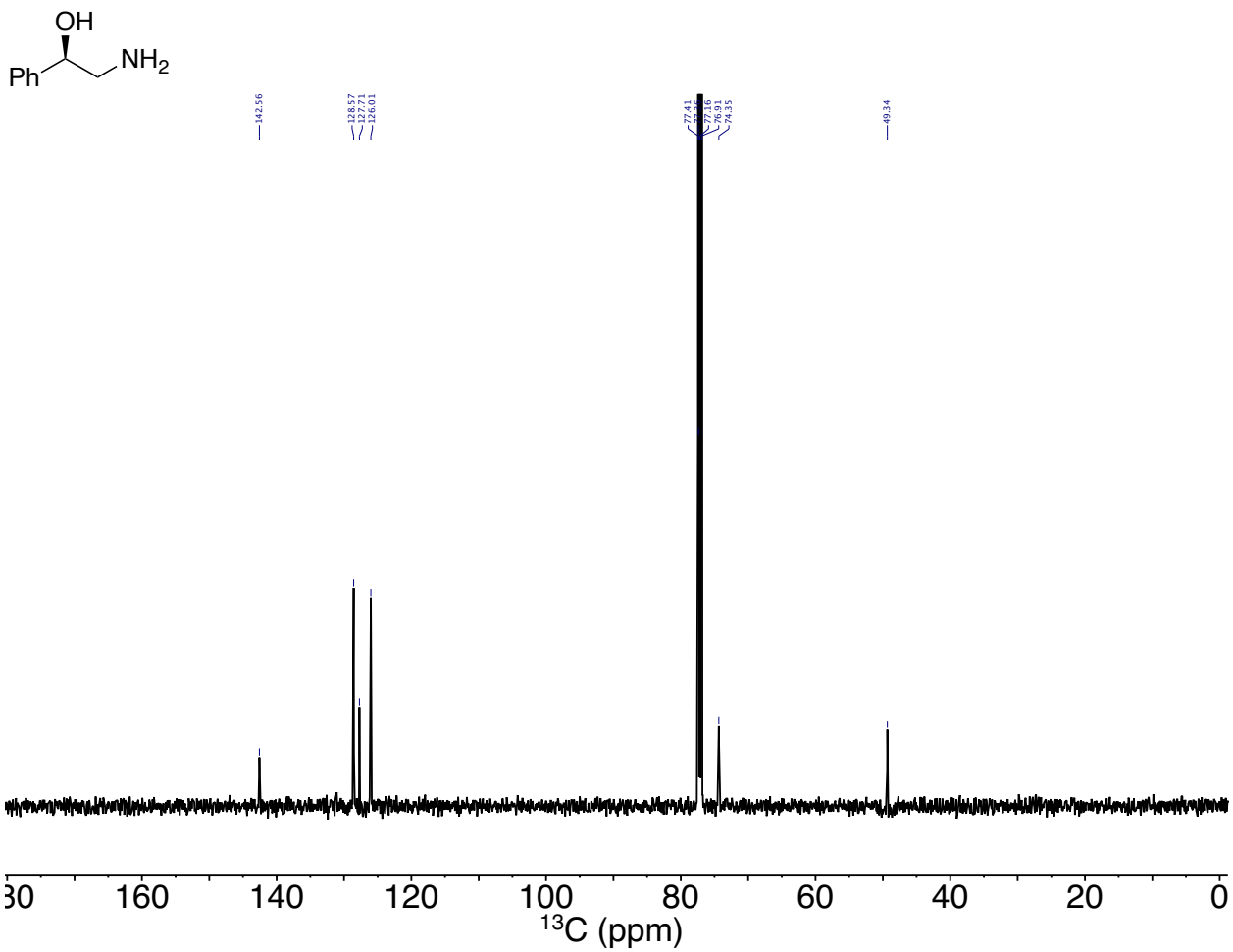
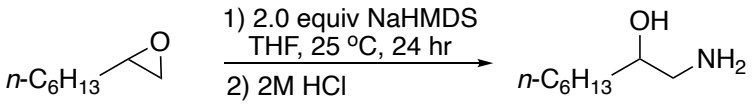


Figure S32. ^{13}C NMR spectrum of (*R*)-2-amino-1-phenylethan-1-ol **29** in $CDCl_3$ at 25 °C.

Synthesis of 1-aminooctan-2-ol 31



Solid sodium hexamethyldisilazide (NaHMDS, 110 mg, 0.6 mmol) was dissolved in 2.0 mL of THF at 25 °C. 2.0 mL of the NaHMDS solution was added to a dry 5.0 mL Kimble vial equipped with a magnetic stir bar. 46 µL of 2-hexyloxirane **30** (0.30 mmol) was then added to the reaction solution. The reaction was stirred at 25 °C for 24 hr. 2M HCl aqueous solution was added to adjust pH = 1, which then was stirred at 25 °C for 24 hr. Saturated NaOH solution was then added until pH = 12. Biphasic mixture was partitioned between water (1.0 mL) and chloroform (5.0 mL). The aqueous layer was separated and extracted further with three 5.0 mL portions of chloroform. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (30% methanol in dichloromethane) afforded 33 mg (76%) of product 1-aminooctan-2-ol **31** as white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 3.5 (dp, J = 7.9, 3.9 Hz, 1H), 2.8 (d, J =12.5 Hz, 1H), 2.5 (dd, J = 12.6, 8.4 Hz, 1H), 2.2 (s, 3H), 1.42 (m, 2H), 1.3 (m, 8H), 0.9 (t, J = 6.2 Hz, 3H).

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 71.9, 47.3, 34.8, 31.8, 29.4, 25.7, 22.6, 14.1.

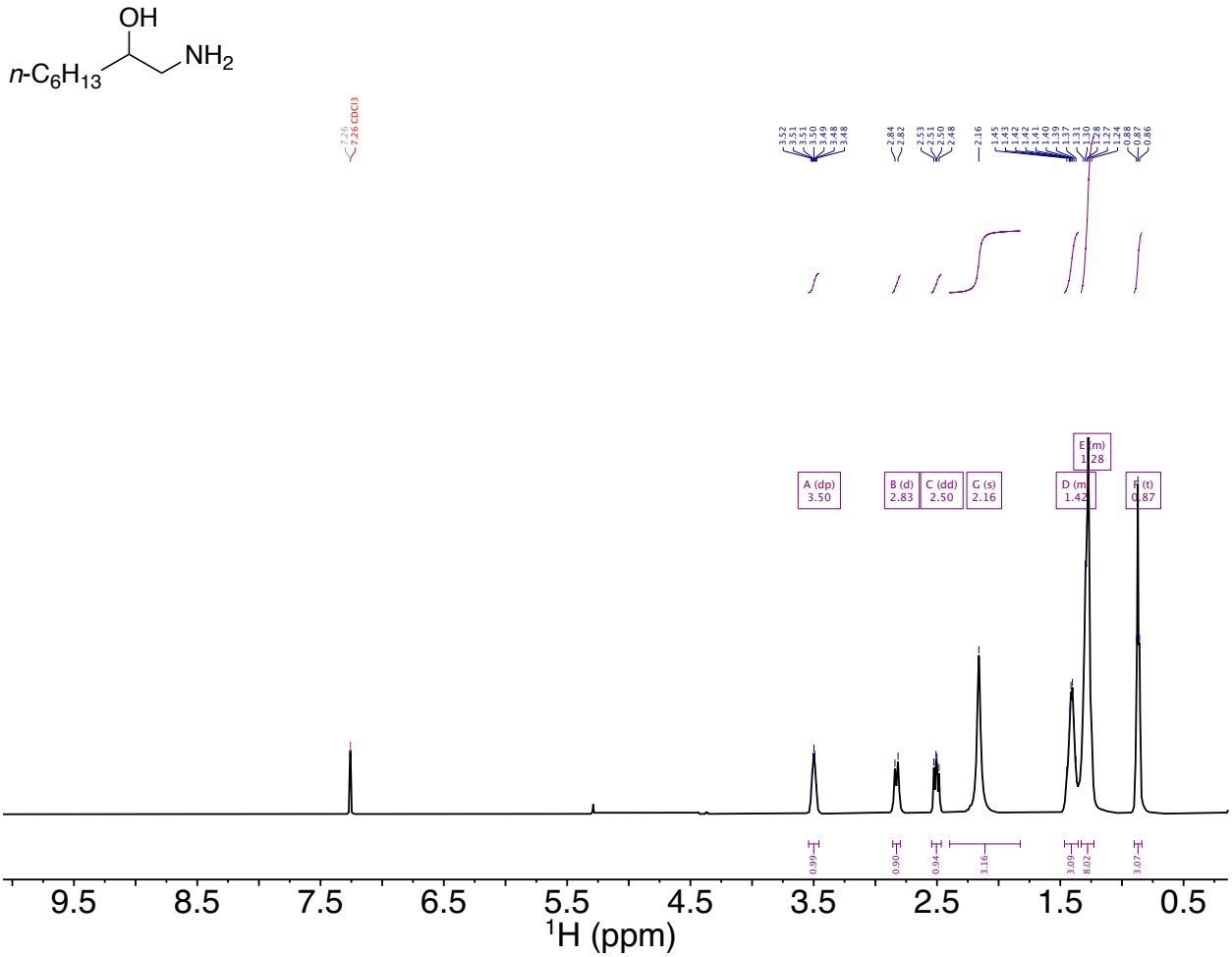


Figure S33. ^{1}H NMR spectrum of 1-aminooctan-2-ol **31** in $CDCl_3$ at 25 °C.

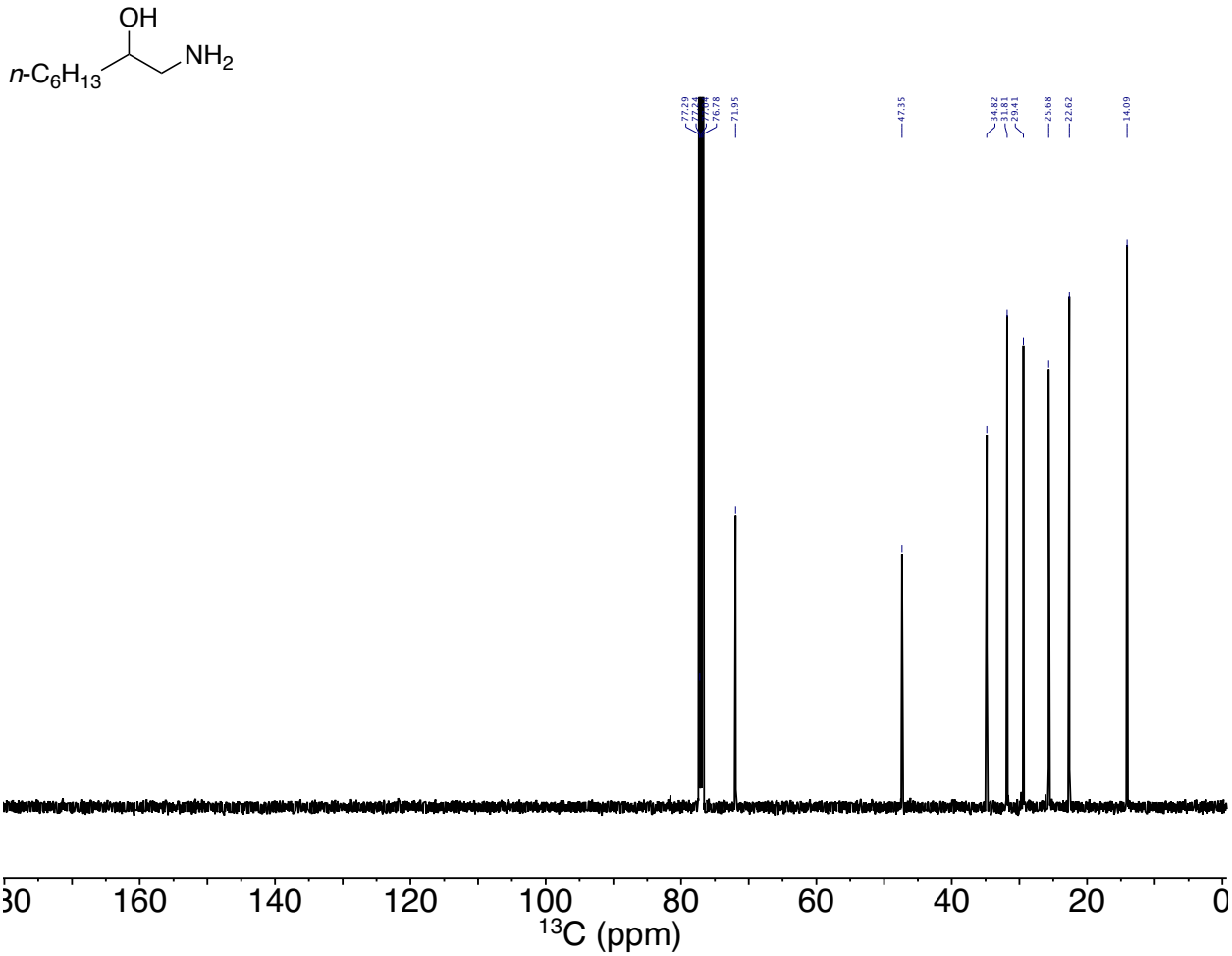


Figure S34. ^{13}C NMR spectrum of 1-aminooctan-2-ol **31** in $CDCl_3$ at 25 °C.

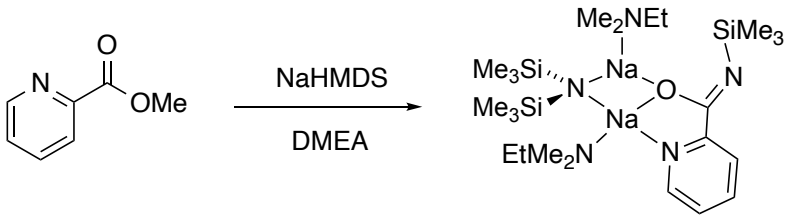
Structural Elucidation and Reaction Mechanism

General procedure for sealed tube NMR spectroscopy

A double-stoppered NMR tube under vacuum was flame-dried on a Schlenk line and allowed to passively cool to room temperature. It was then backfilled with argon and placed in a dry ice/acetone cooling bath. Individual stock solutions of methyl picolinate (**3**) and [^{15}N]NaHMDS were prepared at room temperature. The appropriate amounts of methyl picolinate (**3**), picolinonitrile (**6**), [^{15}N]NaHMDS, solvent, and (when applicable) co-solvent were added sequentially via gastight syringe. Some tubes were flame-sealed under partial vacuum while cold to minimize evaporation and some did not. The tubes were mixed on a vortex mixer and stored at –80 °C.

Standard ^{1}H, ^{13}C, and ^{29}Si direct detection spectra were recorded on a 11.8 T spectrometer at 500.1, 125.8, and 99.3 MHz, respectively. ^{1}H, ^{13}C, and ^{29}Si resonances are referenced to standard TMS. ^{1}H spectra recorded in protonated DMEA and THF solvents were acquired using a WET solvent suppression sequence, whereas the ^{29}Si spectra were acquired utilizing the INEPT sequence.

Integration of the NMR signals were determined using the line-fitting method included in MNova (Mestrelab research S.L.).



46

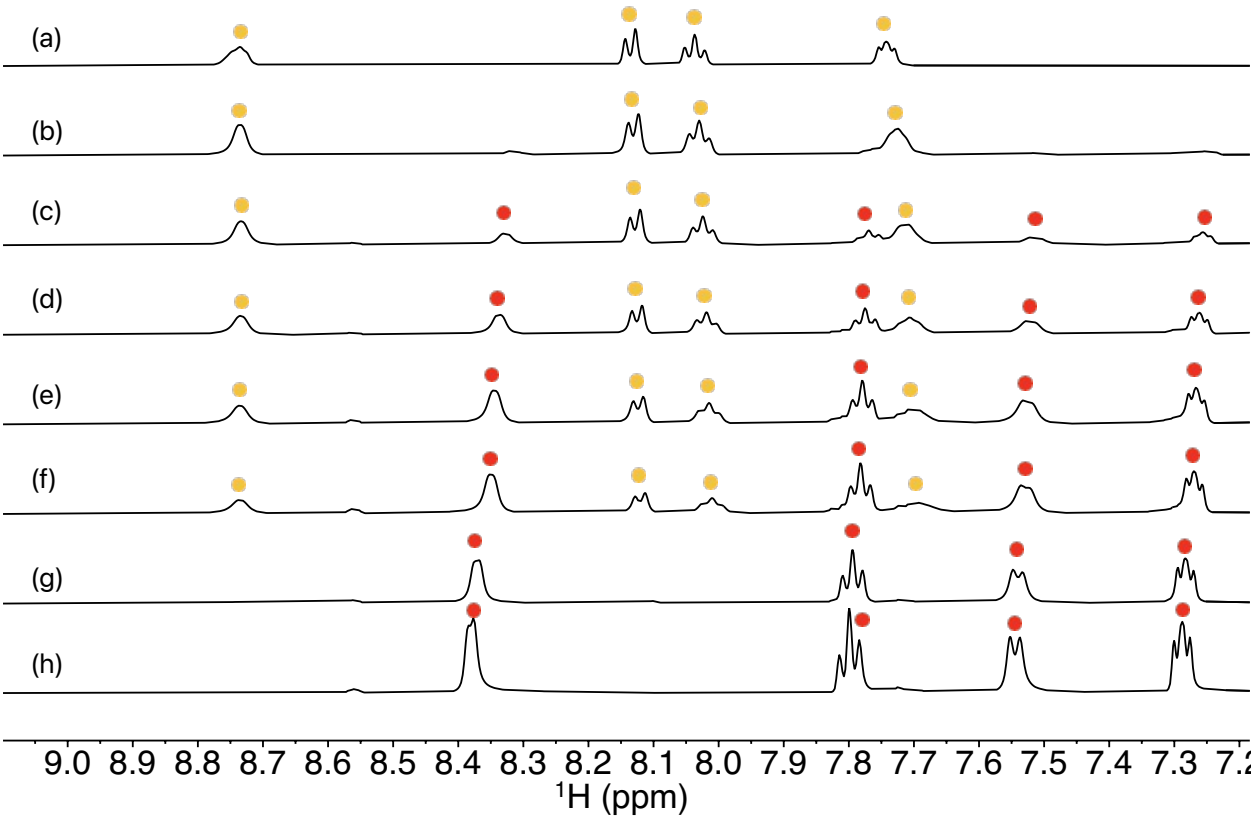


Figure S35. ^{1}H NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **7** and 0.10 M [^{15}N]NaHMDS in DMEA reacting at 25 ºC, observed at a low temperature of –80 ºC. The reaction time for each sample is labeled as (a)–(h) and was varied as follows: 0, 60, 120, 180, 240, 300, 600, and 1200 seconds, respectively. Orange (•) represents methyl picolinate **3**, red (•)represents mixed aggregate **46.**

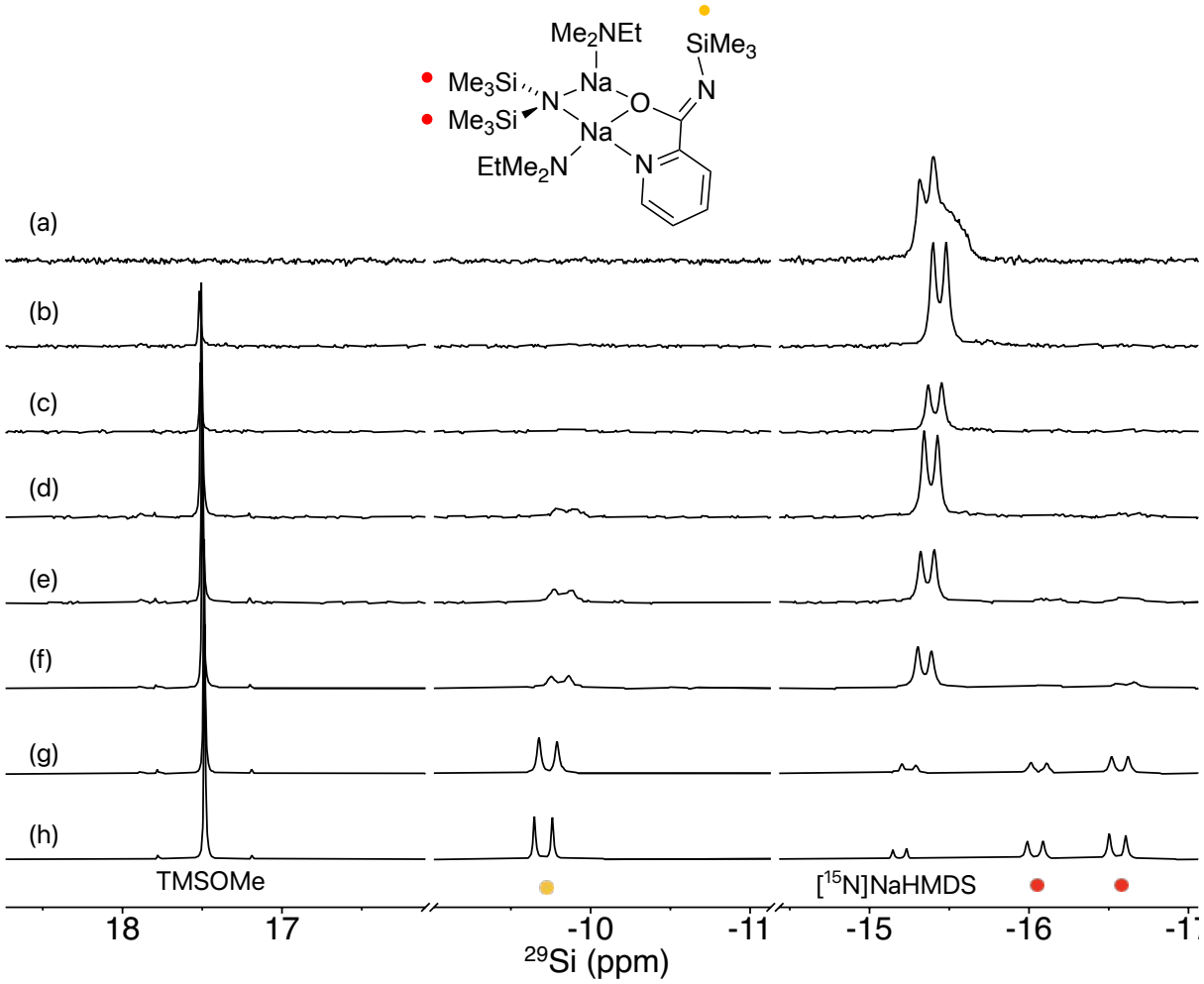


Figure S36. ^{29}Si NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **3** and 0.10 M [^{15}N]NaHMDS in DMEA at 25 °C, observed at a low temperature of –80 °C. The reaction time for each sample is labeled as (a)–(h) and was varied as follows: 0, 60, 120, 180, 240, 300, 600, and 1200 seconds, respectively. Orange (•) represents the *O*-sodium-imino TMS (δ = –9.70 ppm, $J_{N\text{-}Si}$ = 11.2 Hz), red (•)represents the [^{15}N]NaHMDS TMS (δ = –16.04 ppm, $J_{N\text{-}Si}$ = 9.7 Hz and δ = –16.55 ppm, $J_{N\text{-}Si}$ = 10.3 Hz) in mixed aggregate **46.**

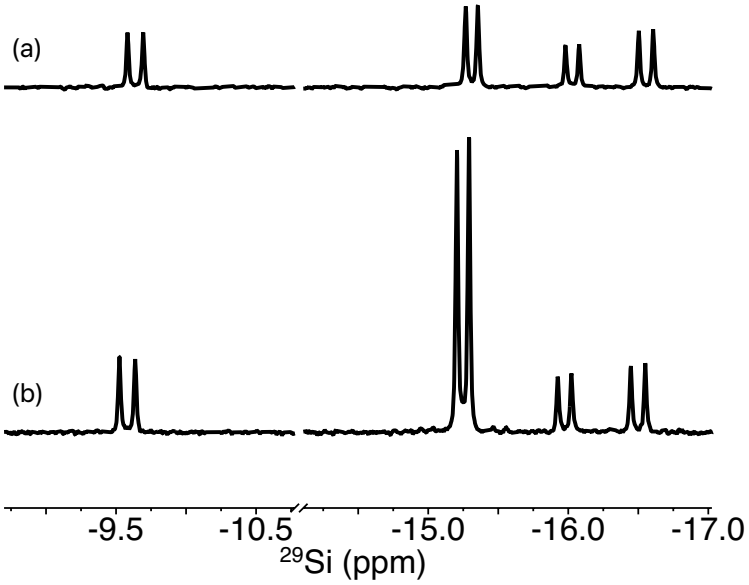


Figure S37. (a) ^{29}Si NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **3** and 0.10 M [^{15}N]NaHMDS in DMEA, within a sealed NMR tube for a period of 30 minutes at 25 ºC, observed at –110 ºC. (b) ^{29}Si NMR spectra of an additional 1 equiv of [^{15}N]NaHMDS added to the reaction mixture (a), observed at –110 ºC.

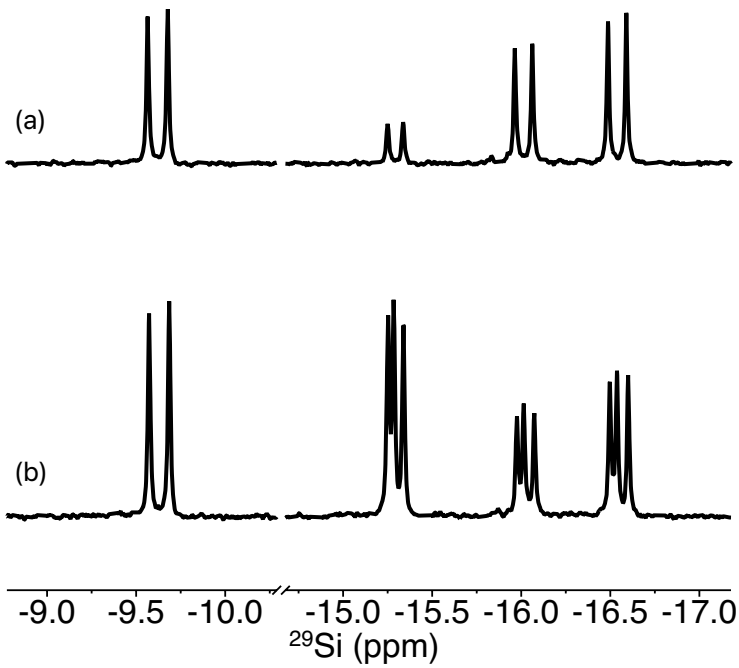


Figure S38. (a) ^{29}Si NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **3** and 0.10 M [^{15}N]NaHMDS in DMEA, within a sealed NMR tube for a period of 30 minutes at 25 ºC, observed at –110 ºC. (b) ^{29}Si NMR spectra of an additional 1.0 equiv of [^{14}N]NaHMDS added to the reaction mixture (a), observed at –110 ºC.

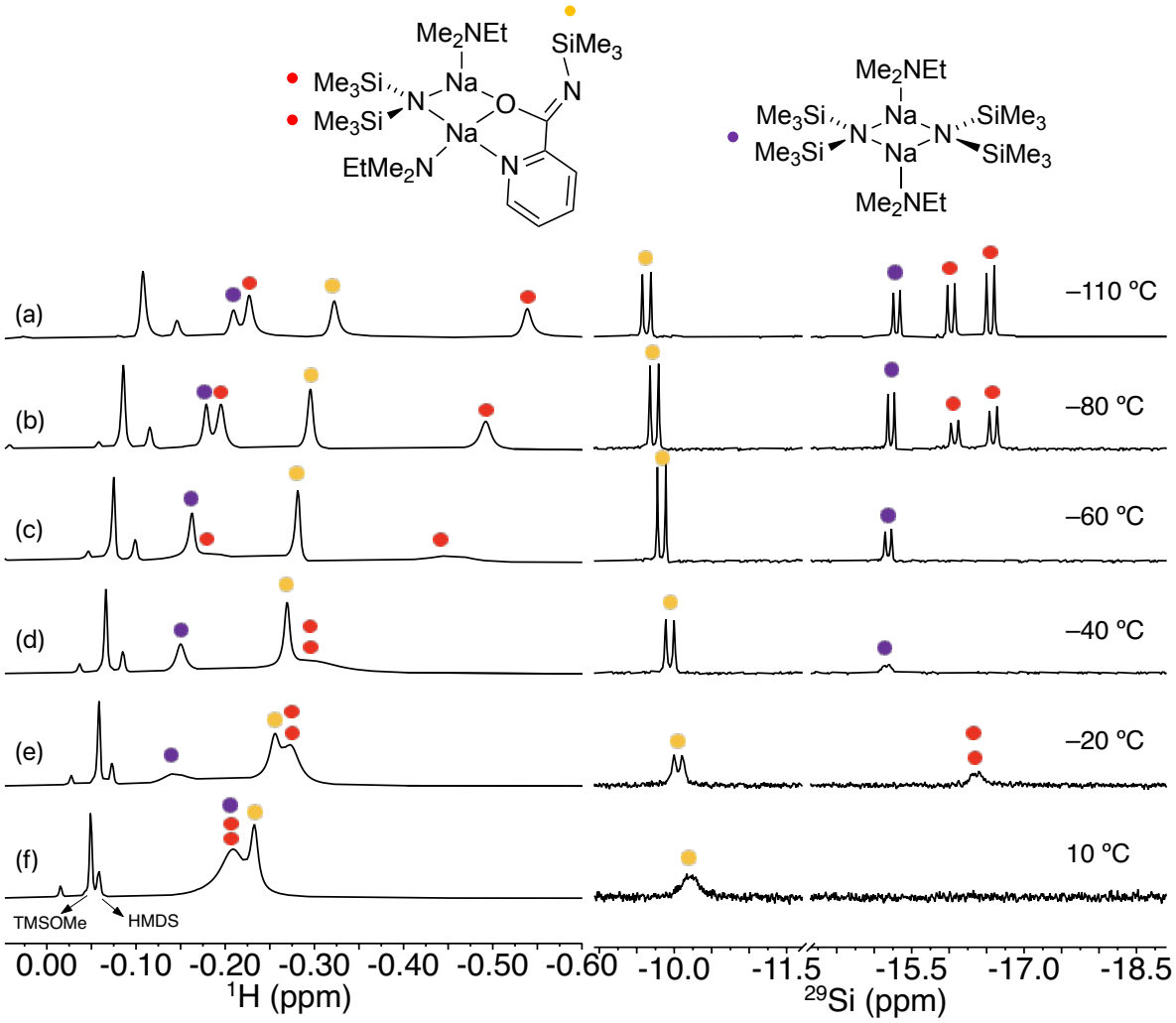


Figure S39. ^{1}H and ^{29}Si NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **3** and 0.10 M [^{15}N]NaHMDS in DMEA within a sealed NMR tube for a period of 30 minutes at 25 °C. The spectra were recorded at different temperatures, as follows: –110 °C, –80 °C, –60 °C, –40 °C, –20 °C and 10 °C, labeled as (a)–(f), respectively. The orange color (•) represents the *O*-sodium-imino TMS signals at δ –9.70 ppm, $J_{N\text{-}Si}$ = 11.2 Hz, while the red color (•) corresponds to the two [^{15}N]NaHMDS TMS signals at δ –16.04 ppm, $J_{N\text{-}Si}$ = 9.7 Hz and δ –16.55 ppm, $J_{N\text{-}Si}$ = 10.3 Hz in mixed aggregate **43**. The purple color (•) indicates the free [^{15}N]NaHMDS.

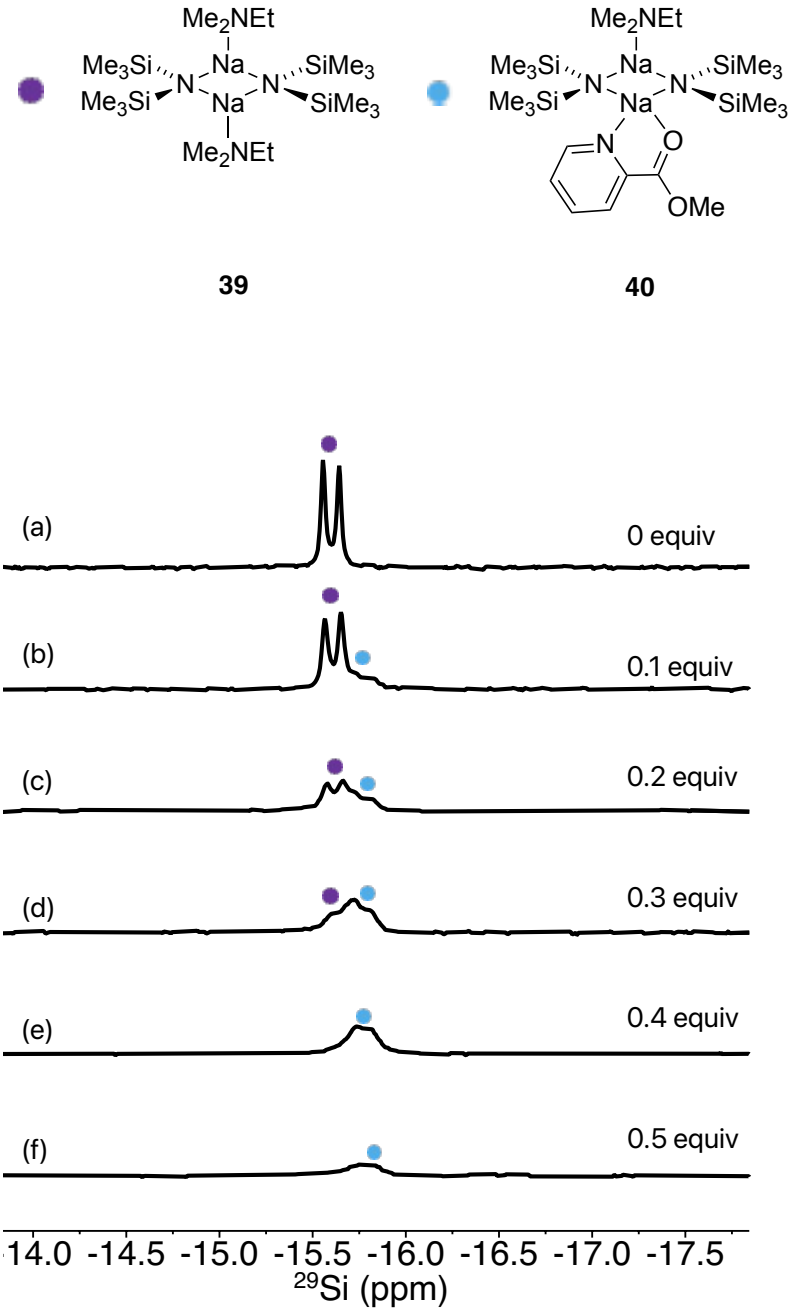
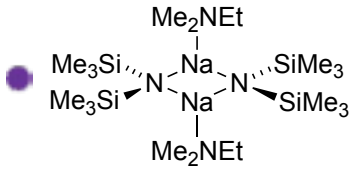
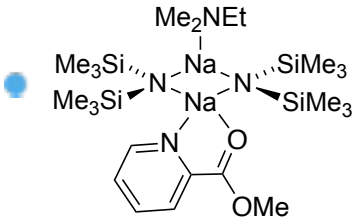


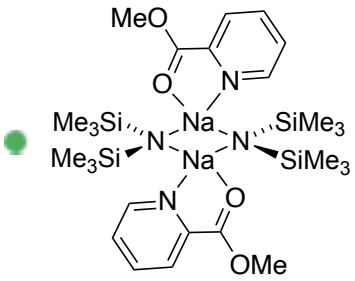
Figure S40. ^{29}Si NMR spectra of 0.10 M [^{15}N]NaHMDS in DMEA at –110 °C with incremental additions of methyl picolinate **3** in DMEA:pentane = 1:2 at –78 °C. The equiv of total added substrate for (a) to (f) are as follows: 0.0, 0.1, 0.2, 0.3, 0.4 and 0.5 respectively. ^{29}Si spectra are referenced to a TMS internal standard (0.00 ppm).


Me2NEt
Me3Si
N
Na
N
SiMe3
Me3Si
Na
SiMe3
Me2NEt

39


Me2NEt
Me3Si
N
Na
N
SiMe3
Me3Si
Na
SiMe3
N
O
OMe

40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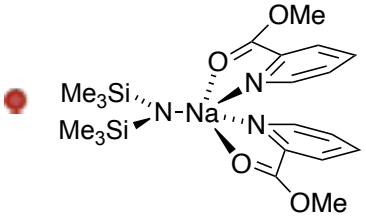
Na
N
SiMe3
Me3Si
Na
SiMe3
N
O
OMe

41


OMe
O
N
Me3Si
N-Na
N
Me3Si
O
OMe

42

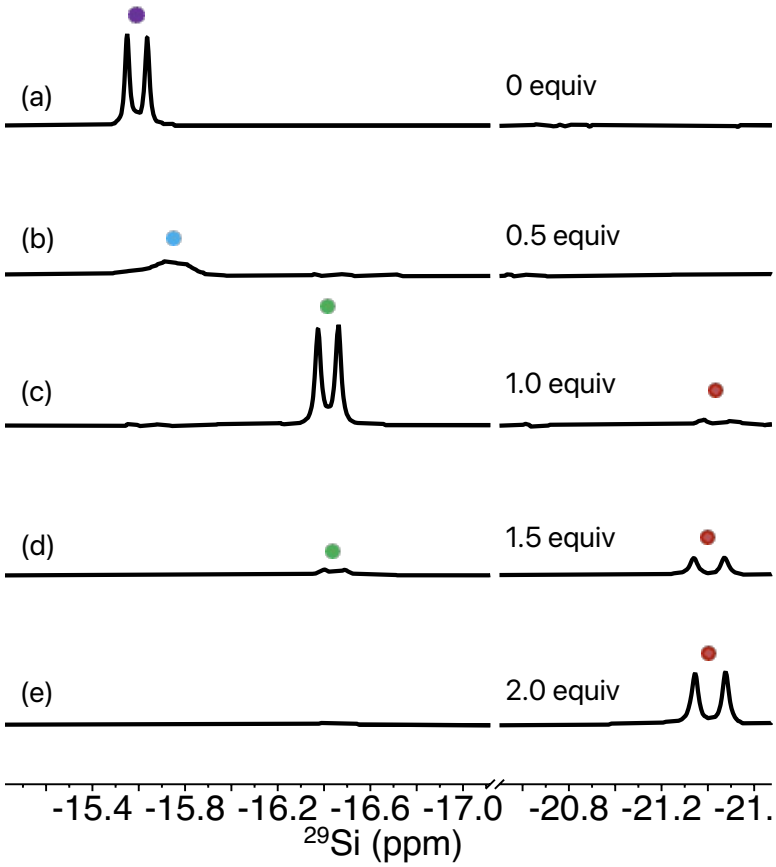


Figure S41. ^{29}Si NMR spectra of 0.10 M [^{15}N]NaHMDS in DMEA at –110 °C with incremental additions of methyl picolinate **3** in DMEA:pentane = 2:1 at –78 °C. The equiv of total added substrate for (a) to (e) are as follows: 0.0, 0.5, 1.0, 1.5 and 2.0 respectively. ^{29}Si spectra are referenced to a TMS internal standard (0.00 ppm).

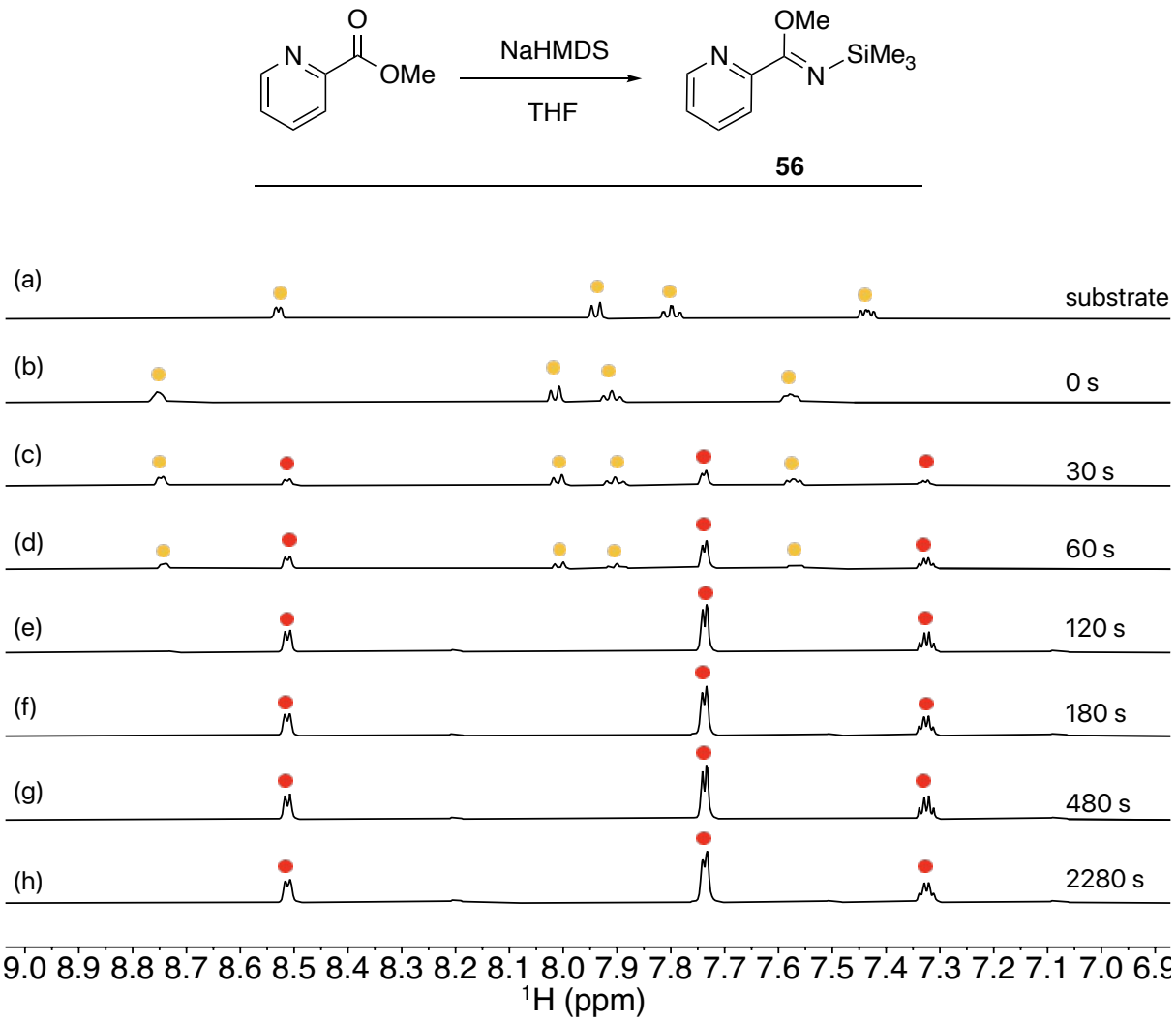


Figure S42. ^{1}H NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **3** and 0.10 M [^{15}N]NaHMDS in THF reacting at 25 °C, observed at –110 °C. Reaction times for (a)–(h) are as follows: only susbtrate (without base), 0, 30, 60, 120, 180, 480 and 2280 s, respectively. ^{29}Si spectra are referenced to a TMS internal standard (0.00 ppm). Orange (•) represents methyl picolinate **3**, red (•) represents imino ether **56.**

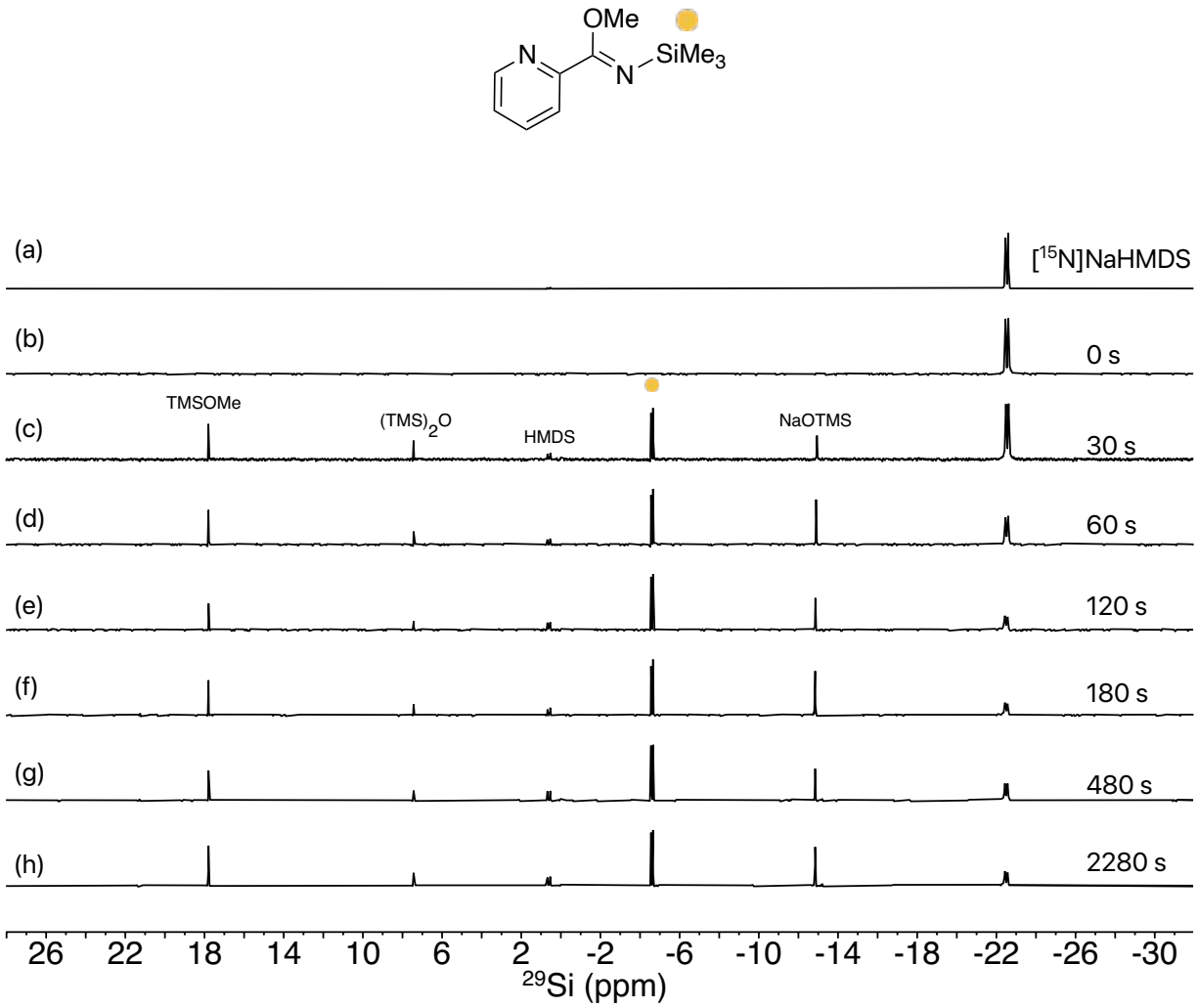


Figure S43. ^{29}Si NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **3** and 0.10 M [^{15}N]NaHMDS in THF reacting at 25 ºC, observed at –110 ºC. Reaction times for (a)–(h) are as follows: only [^{15}N]NaHMDS, 0, 60, 120, 180, 480 and 2280 s, respectively. Orange (•)represents the TMS of *O*-methyl-imino ether **56** (δ –4.61 ppm, $J_{N\text{-}Si}$ = 10.0 Hz).

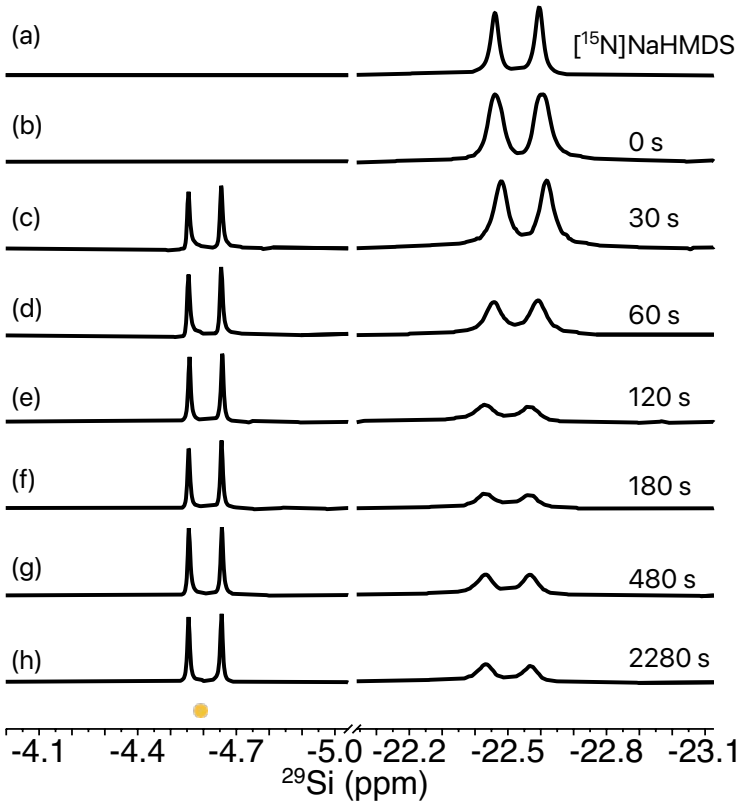


Figure S44. ^{29}Si NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **3** and 0.10 M [^{15}N]NaHMDS in THF reacting at 25 ºC, observed at –110 ºC. Reaction times for (a)–(h) are as follows: only [^{15}N]NaHMDS, 0, 60, 120, 180, 480 and 2280 s, respectively. ^{29}Si spectra are referenced to a TMS internal standard (0.00 ppm). Orange (•)represents the TMS of *O*-methyl-imino ether **56** (δ –4.51 ppm, $J_{N\text{-}Si}$ = 10.0 Hz).

Crude mixture of imino ether 56

Solid sodium hexamethyldisilazide (NaHMDS, 165 mg, 0.9 mmol) was dissolved in 2.0 mL of tetrahydrofuran (THF) at room temperature. Subsequently, 2.0 mL of the resulting NaHMDS solution was introduced into a dry 5.0 mL Kimble vial fitted with a magnetic stir bar. To the reaction solution, 36 µL of methyl picolinate (0.30 mmol) was added, and the resulting mixture was stirred at 25 °C for 0.3 hours. The reaction was then quenched using 10 equiv of water, followed by removal of all solvent by rotary evaporation. The residue was dissolved in $CDCl_3$, and the proton spectrum of the crude mixture was obtained.

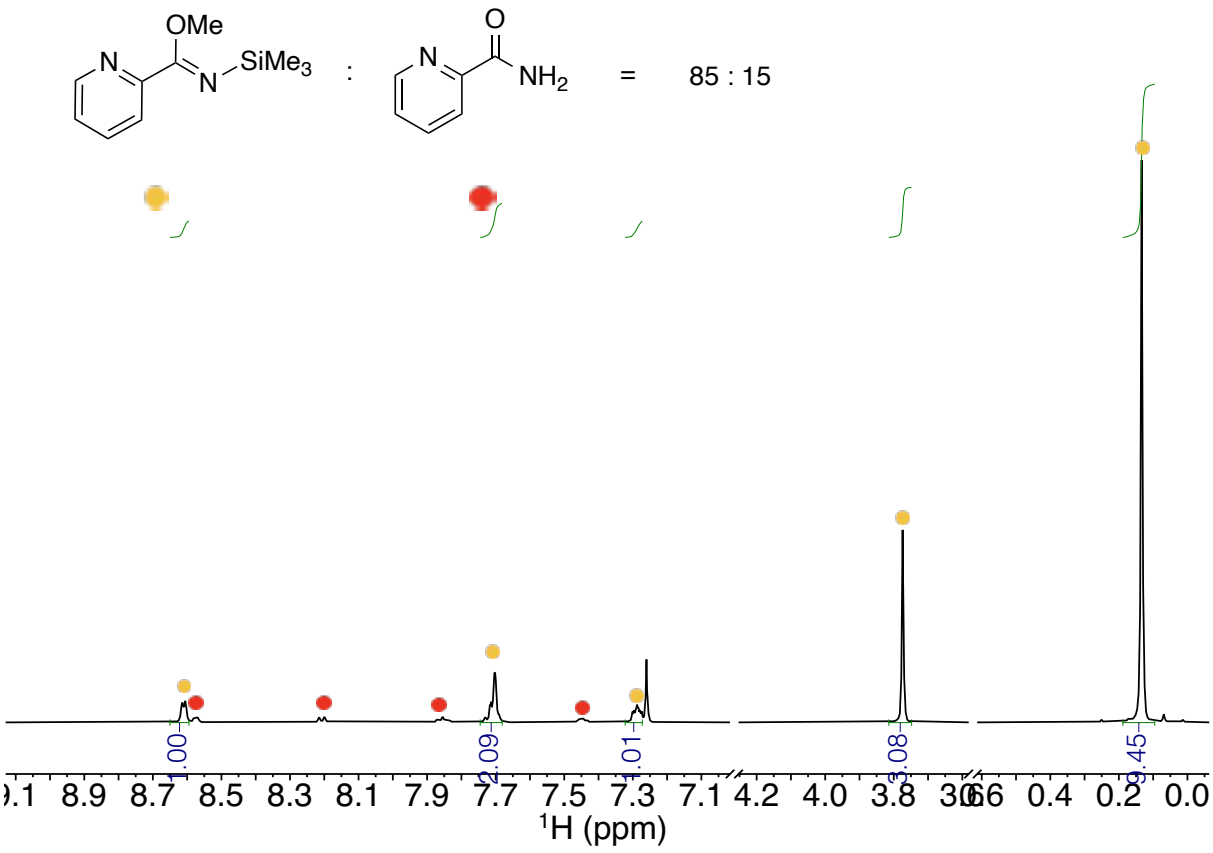


Figure S45. ^1H NMR spectra of crude mixture in $CDCl_3$. Orange (●) represents imino ether **28**, red (●) represents carboxamide **4.**

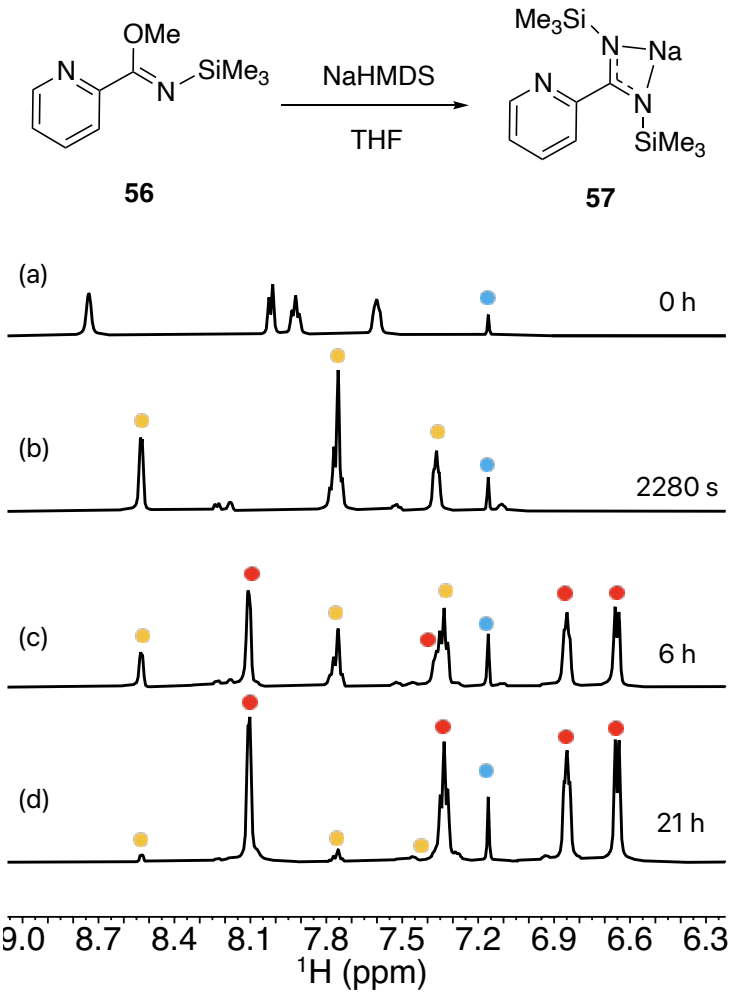


Figure S46. ^{1}H NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **7** and 0.15 M [^{15}N]NaHMDS in THF reacting at 25 °C, observed at –110 °C. Reaction times for (a)–(d) are as follows: 0 s, 2280 s, 6 h, 21 h, respectively. Orange (●) represents the *O*-methyl-imino **56**. ^{1}H spectra are referenced to a TMS internal standard (0.00 ppm). Red (●) represents silyated amidine **57**. Blue (●) represents benzene from Na / benzophenone still.

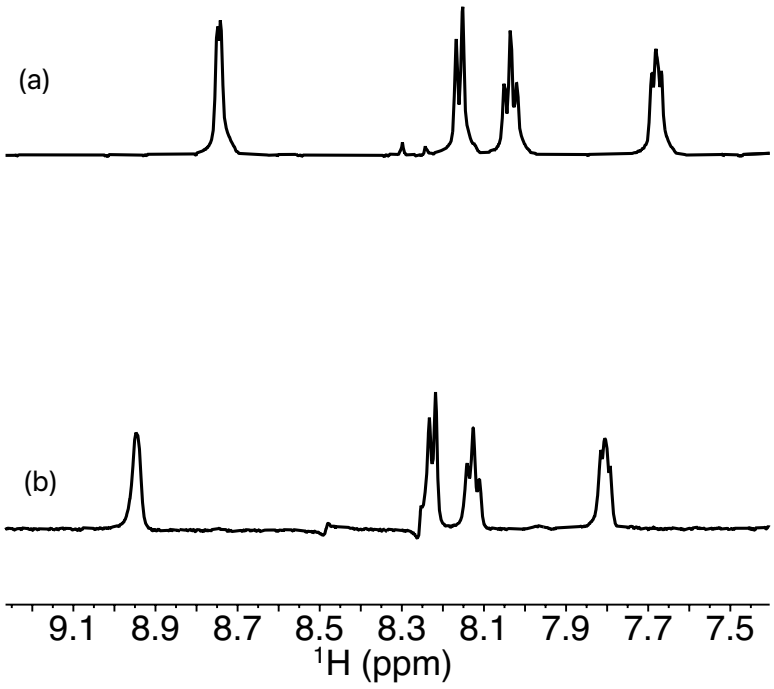


Figure S47. (a)^{1}H NMR spectra of 0.050 M methyl picolinate **3** in THF, observed at –110 ºC (b)^{1}H NMR spectra of 0.050 M methyl picolinate **3** and 0.15 M [^{15}N]NaHMDS in THF before reaction, observed at –110 ºC. ^{1}H spectra are referenced to a TMS internal standard (0.00 ppm).

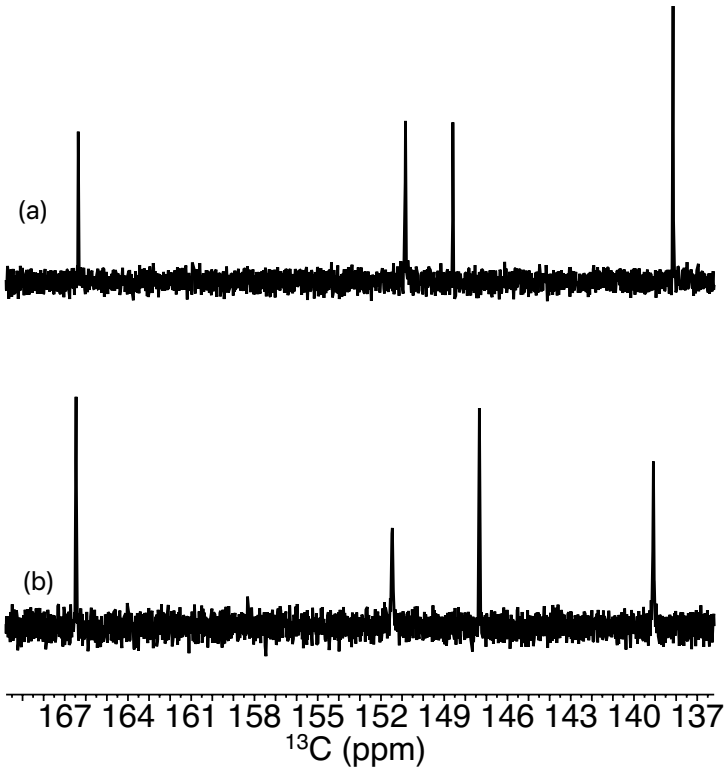


Figure S48. (a) ^{13}C NMR spectra of 0.050 M methyl picolinate **3** in THF, observed at –110 ºC (b) ^{13}C NMR spectra of 0.050 M methyl picolinate **3** and 0.15 M [^{15}N]NaHMDS in THF before reaction, observed at –110 ºC. ^{13}C spectra are referenced to a TMS internal standard (0.00 ppm).

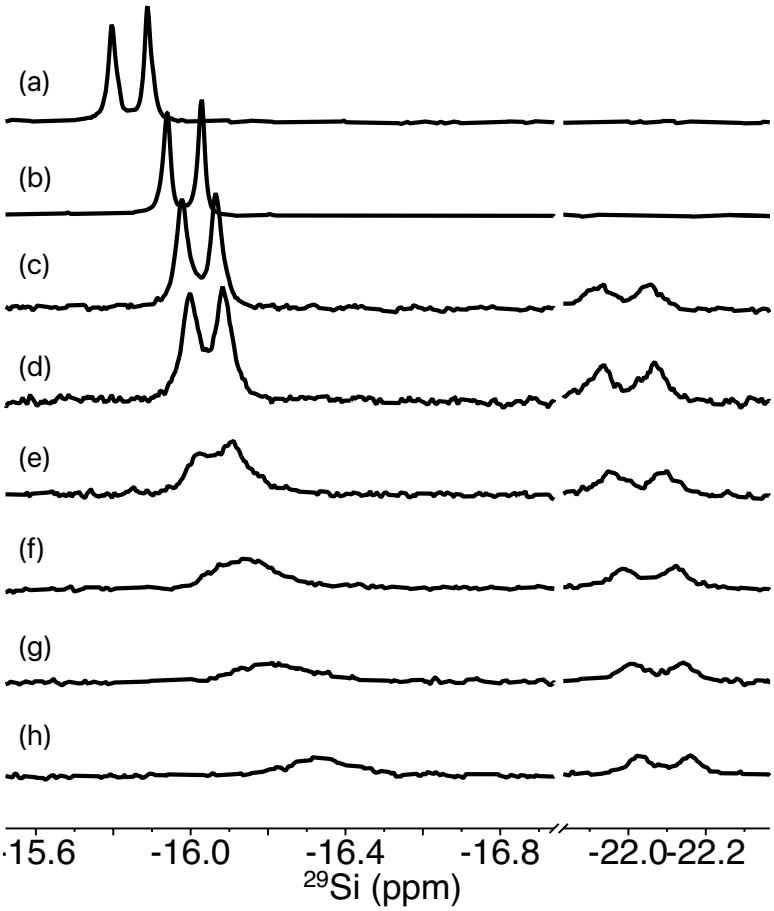


Figure S49. (a)–(c) ^{29}Si NMR spectra of 0.10 M [^{15}N]NaHMDS in DMEA at –110 °C with incremental additions of THF. The equiv of THF for (a) to (c) are as follows: 0.0, 2.0, and 4.0 respectively. (d)–(h) ^{29}Si NMR spectra are followed incremental additions of methyl picolinate **3** in DMEA:pentane = 1:2 solvent. The equiv of methyl picolinate **3** for (d) to (h) are as follows: 0.1, 0.2, 0.3, 0.4 and 0.5 respectively. ^{29}Si spectra are referenced to a TMS internal standard (0.00 ppm).

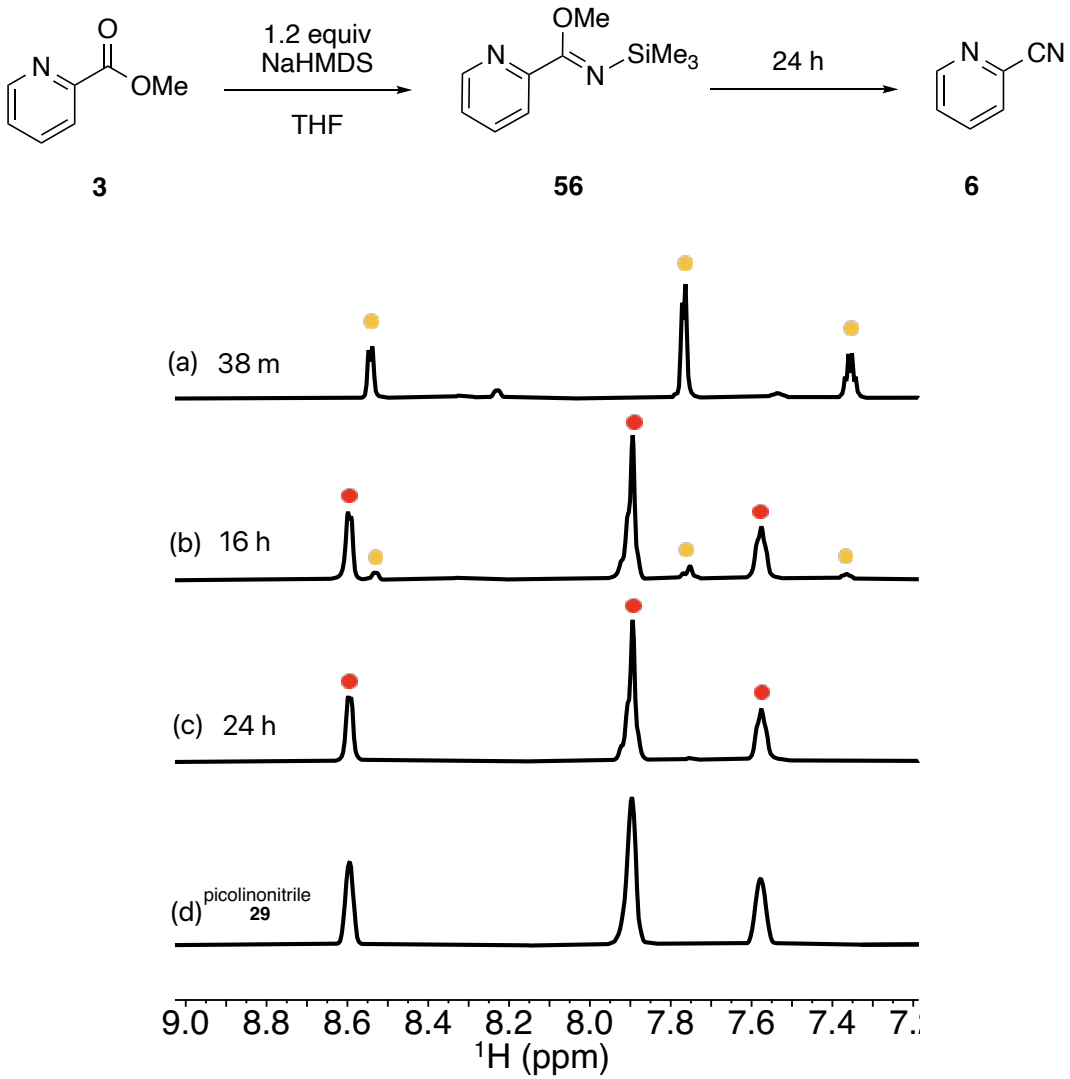


Figure S50. ^{1}H NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **3** and 0.06 M [^{15}N]NaHMDS in THF reacting at 25 °C, observed at –110 °C. Reaction times for spectra (a)–(c) are as follows: 38 m, 16 h, 24 h, respectively. Spectrum (d) corresponds to picolinonitrile **6** sample dissolved in THF. ^{1}H spectra are referenced to a TMS internal standard (0.00 ppm). Orange (•) represents the *O*-methyl-imino ether **56**. Red (•) represents an authentic sample of picolinonitrile **6**.

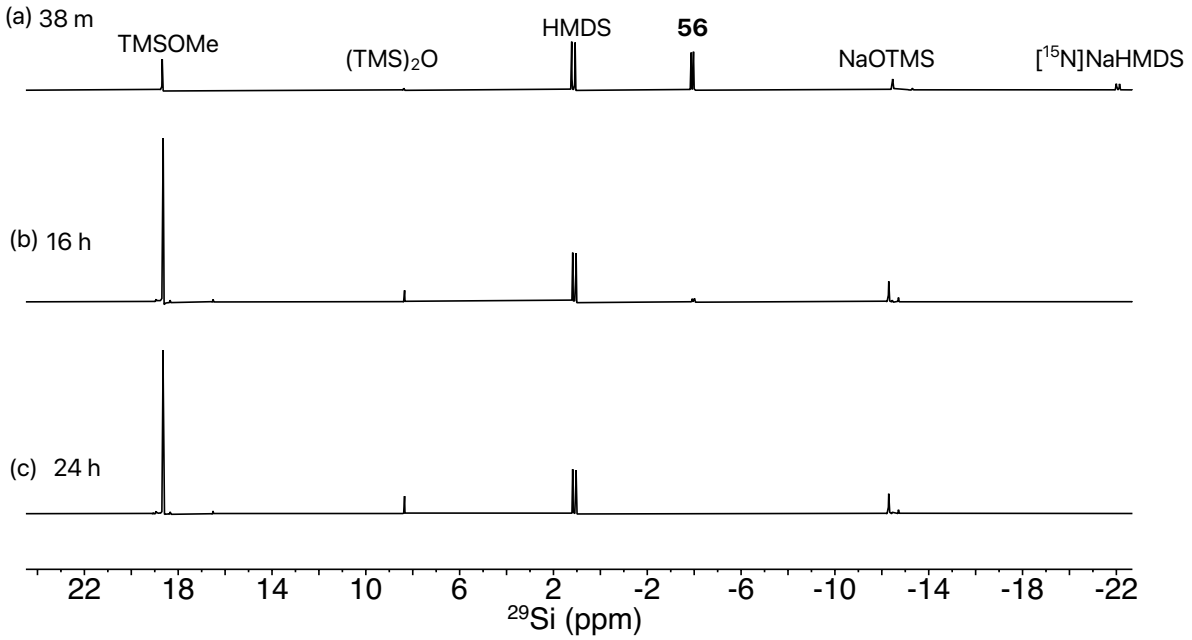


Figure S51. ^{29}Si NMR spectra of a reaction mixture containing 0.050 M methyl picolinate **3** and 0.060 M [^{15}N]NaHMDS in THF at 25 ºC, observed at a low temperature of –110 ºC. Reaction times for spectra (a)–(c) are as follows: 38 m, 16 h, 24 h, respectively.

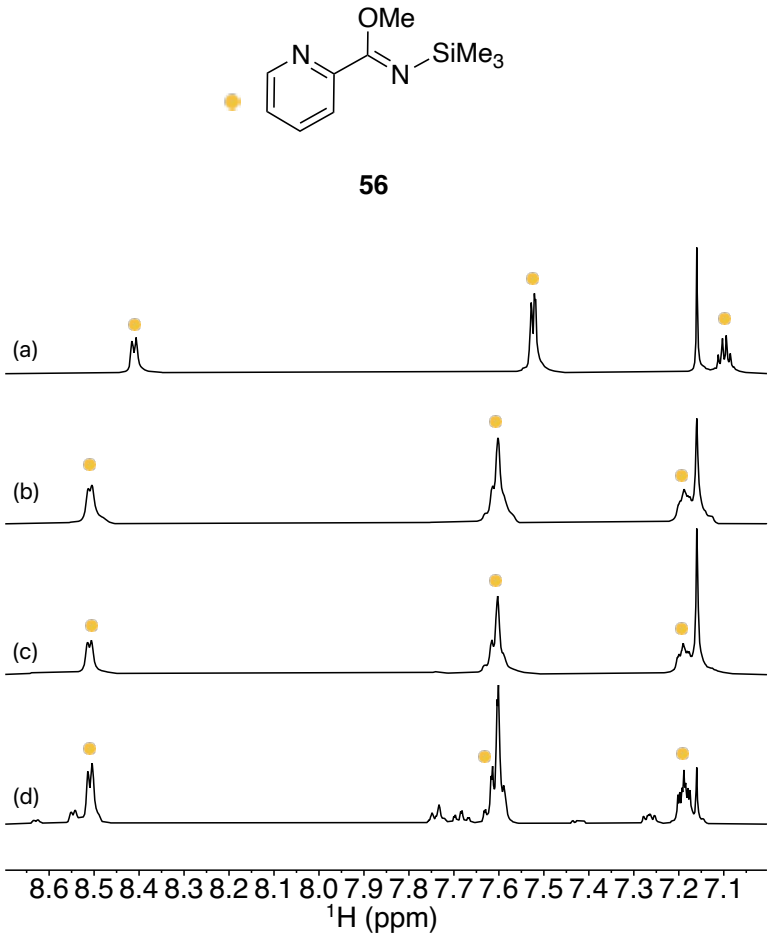
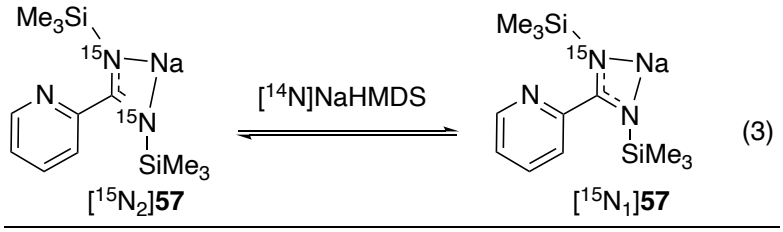


Figure S52. (a) ^{1}H NMR spectrum of crude *O*-methyl-imino ether **56** in $CDCl_3$, observed at 25 ºC. (b) ^{1}H NMR spectrum obtained after the reaction between *O*-methyl-imino ether **56** (*from (a)*) and 1 equiv of NaOMe in THF at 50 ºC for 30 minutes, followed by the evaporation of THF and subsequent dissolution of the resulting product in $CDCl_3$. (c) ^{1}H NMR spectrum obtained after the reaction between *O*-methyl-imino ether **56** (*from (b)*) and 1 equiv of NaOTMS in THF at 50 ºC for 30 minutes, followed by the evaporation of THF and subsequent dissolution of the resulting product in $CDCl_3$. (d) ^{1}H NMR spectrum obtained after the reaction between *O*-methyl-imino ether **55** (*from (c)*) and 0.20 equiv of NaHMDS in THF at 50 ºC for 30 minutes, followed by the evaporation of THF and subsequent dissolution of the resulting product in $CDCl_3$. ^{1}H spectra are referenced to $CDCl_3$ (7.16 ppm).

Virtual coupling of amidine



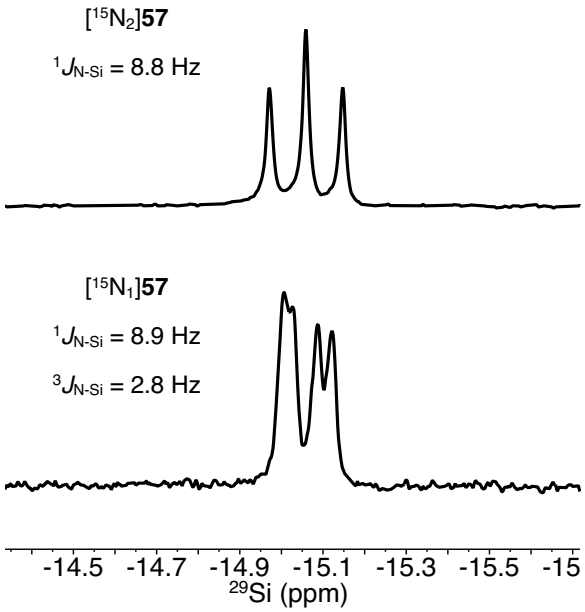


Figure S53. ^{29}Si NMR spectra of [^{15}N$_2$]**56** showing virtual coupling ($J_{N–Si}$ = 8.8 Hz) and standard coupling in [^{15}N$_1$]**56** ($^1J_{N–Si}$ = 8.9 Hz and $^3J_{N–Si}$ = 2.8 Hz).

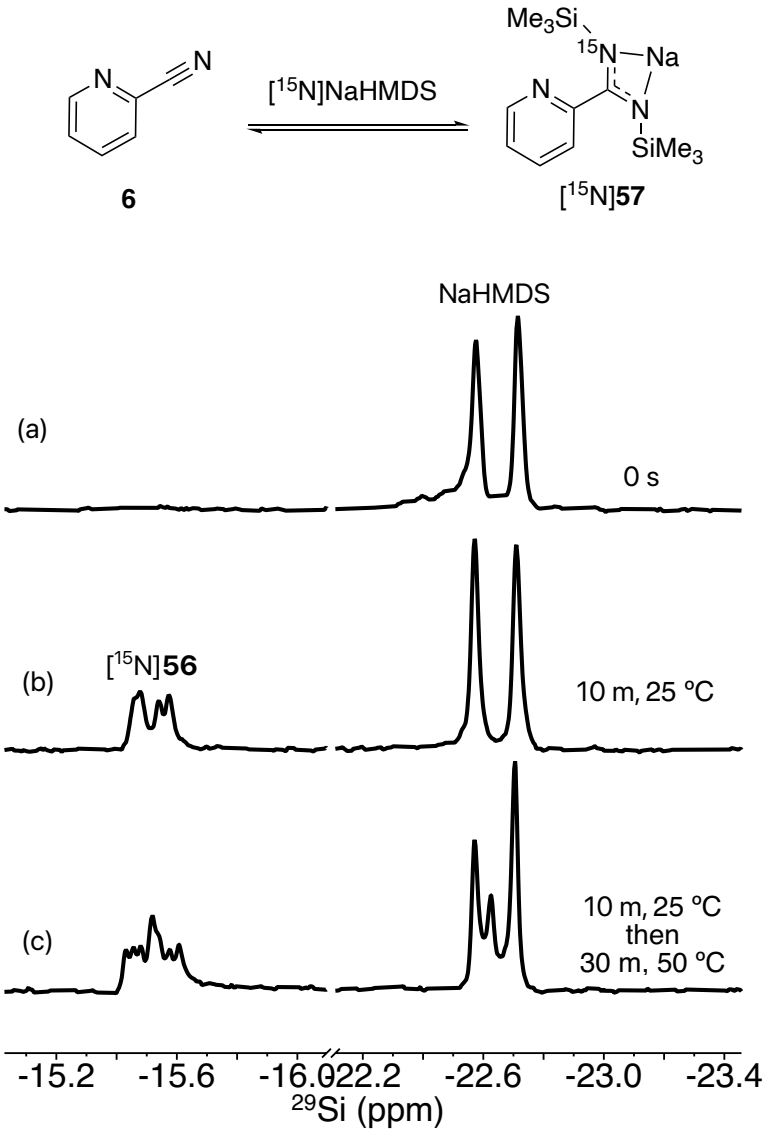


Figure S54. ^{29}Si NMR spectra of a reaction mixture containing 0.050 M picolinonitrile **6** and 0.10 M [^{15}N]NaHMDS in THF, observed at –110 °C. The reaction progress was monitored by analyzing the status of the sealed NMR tube at various reaction times and temperatures. ^{29}Si spectra are referenced to a TMS internal standard (0.00 ppm). Spectra (a)–(c) represent the status of the sealed NMR tube at different reaction times and temperatures. (a) 0 m at 25 °C. (b) 10 m at 25 °C. (c) 10 m at 25 °C, followed by 30 m at 50 °C.

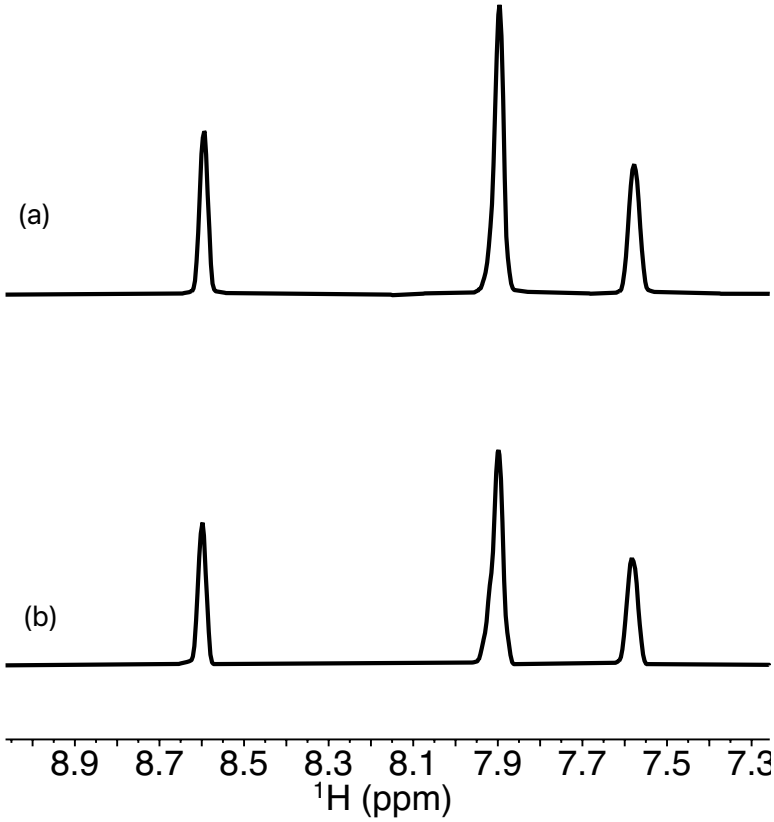


Figure S55. (a) ^{1}H NMR spectrum of 0.050 M picolinonitrile **6** in THF, observed at –110 ºC. (b) ^{1}H NMR spectrum of 0.050 M methyl picolinate **3** and 0.15 M [^{15}N]NaHMDS in THF before reaction, observed at –110 ºC. ^{1}H spectra are referenced to a TMS internal standard (0.00 ppm).

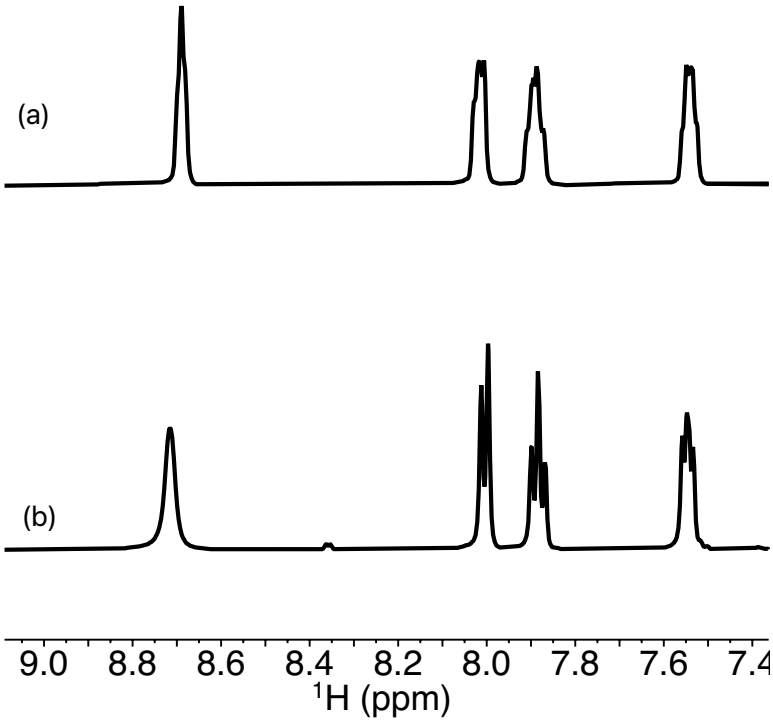


Figure S56. (a) ^{1}H NMR spectra of 0.050 M picolinonitrile **6** in DMEA, observed at –110 ºC. (b) ^{1}H NMR spectra of 0.050 M methyl picolinate **7** and 0.15 M [^{15}N]NaHMDS in DMEA before reaction, observed at –110 ºC. ^{1}H spectra are referenced to a TMS internal standard (0.00 ppm).

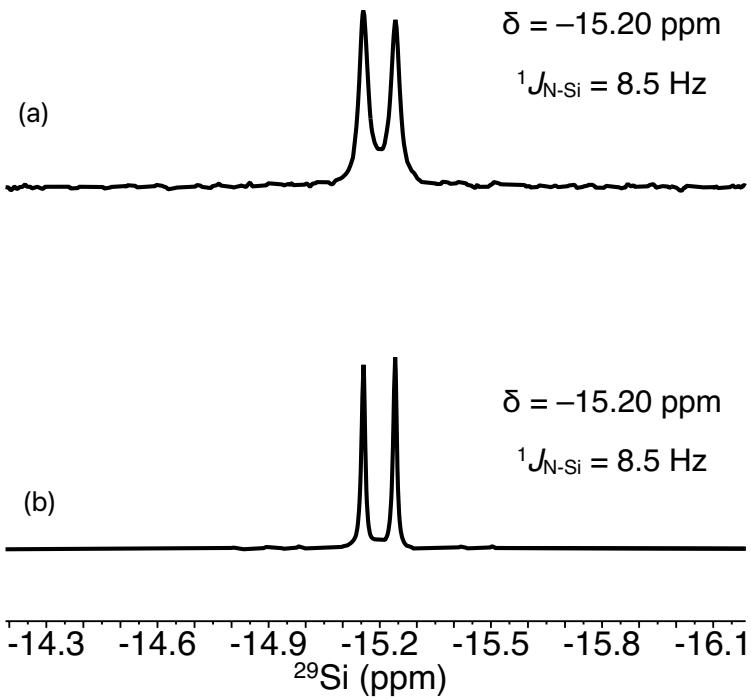


Figure S57. (a) ^{29}Si NMR spectra of 0.050 M picolinonitrile **6** in DMEA, observed at –110 ºC. (b) ^{29}Si NMR spectra of 0.050 M methyl picolinate **3** and 0.15 M [^{15}N]NaHMDS in DMEA before reaction, observed at –110 ºC. ^{1}H spectra are referenced to a TMS internal standard (0.00 ppm).

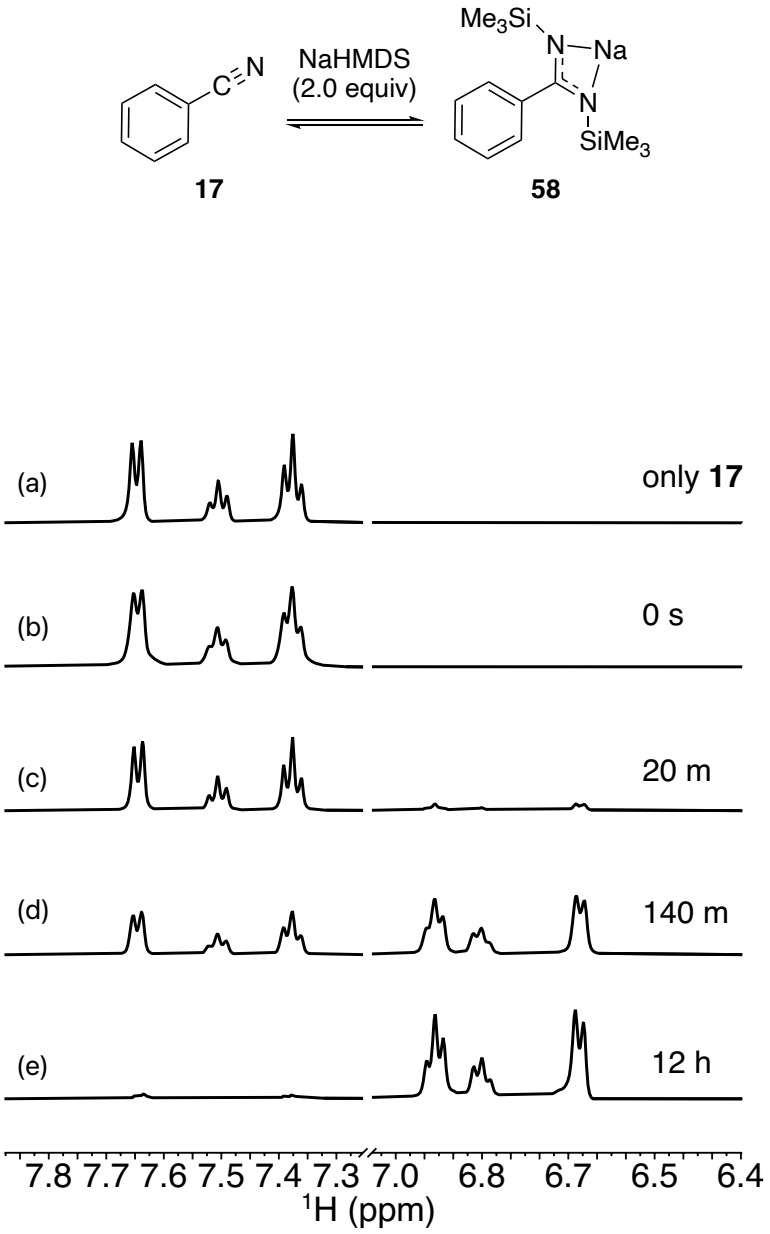


Figure S58. ^{1}H NMR spectra of a reaction mixture containing 0.050 M benzonitrile **17** and 0.10 M [^{15}N]NaHMDS in THF reacting at 25 ºC, observed at –110 ºC. Reaction times for spectra (b)–(e) are as follows: 0 s, 20 m, 140 m and 12 h respectively. Spectrum (a) corresponds to authentic benzonitrile **17** sample dissolved in THF. ^{1}H spectra are referenced to a TMS internal standard (0.00 ppm).

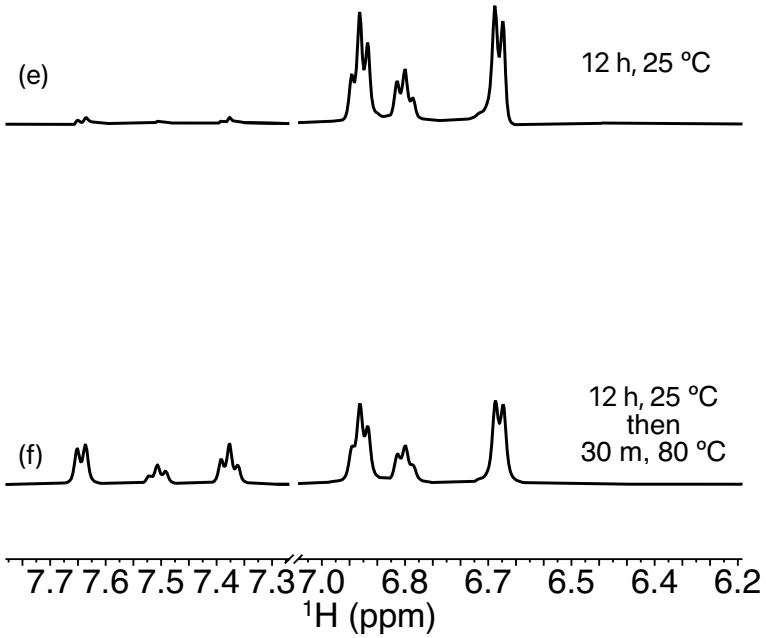
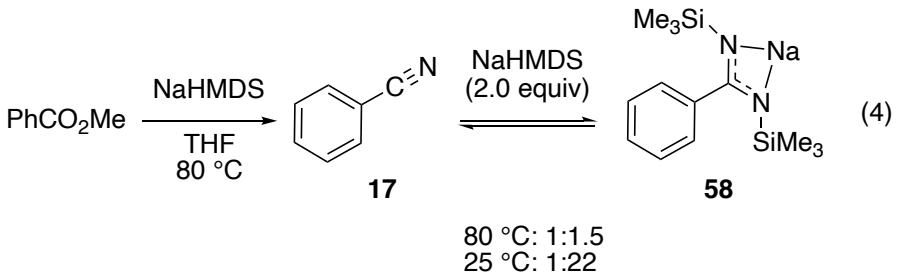


Figure S59. ^{1}H NMR spectra of a reaction mixture containing 0.050 M benzonitrile **17** and 0.10 M [^{15}N]NaHMDS in THF reacting at 25 ºC and 80 ºC, observed at –110 ºC. The reaction mixture is the same as of **Figure S58**. Spectrum (e) is the same spectrum in **Figure S58**. After reacting at 80 ºC for 30 min, the NMR tube containing the reaction mixture was immediately put into a dry ice acetone bath, and spectrum (f) was taken. Spectra (e) and (f) represent the status of the sealed NMR tube at different reaction times and temperatures. (e) 12 h at 25 ºC, (f) 12 h at 25 ºC, followed by 30 m at 80 ºC.^{1}H spectra are referenced to a TMS internal standard (0.00 ppm).



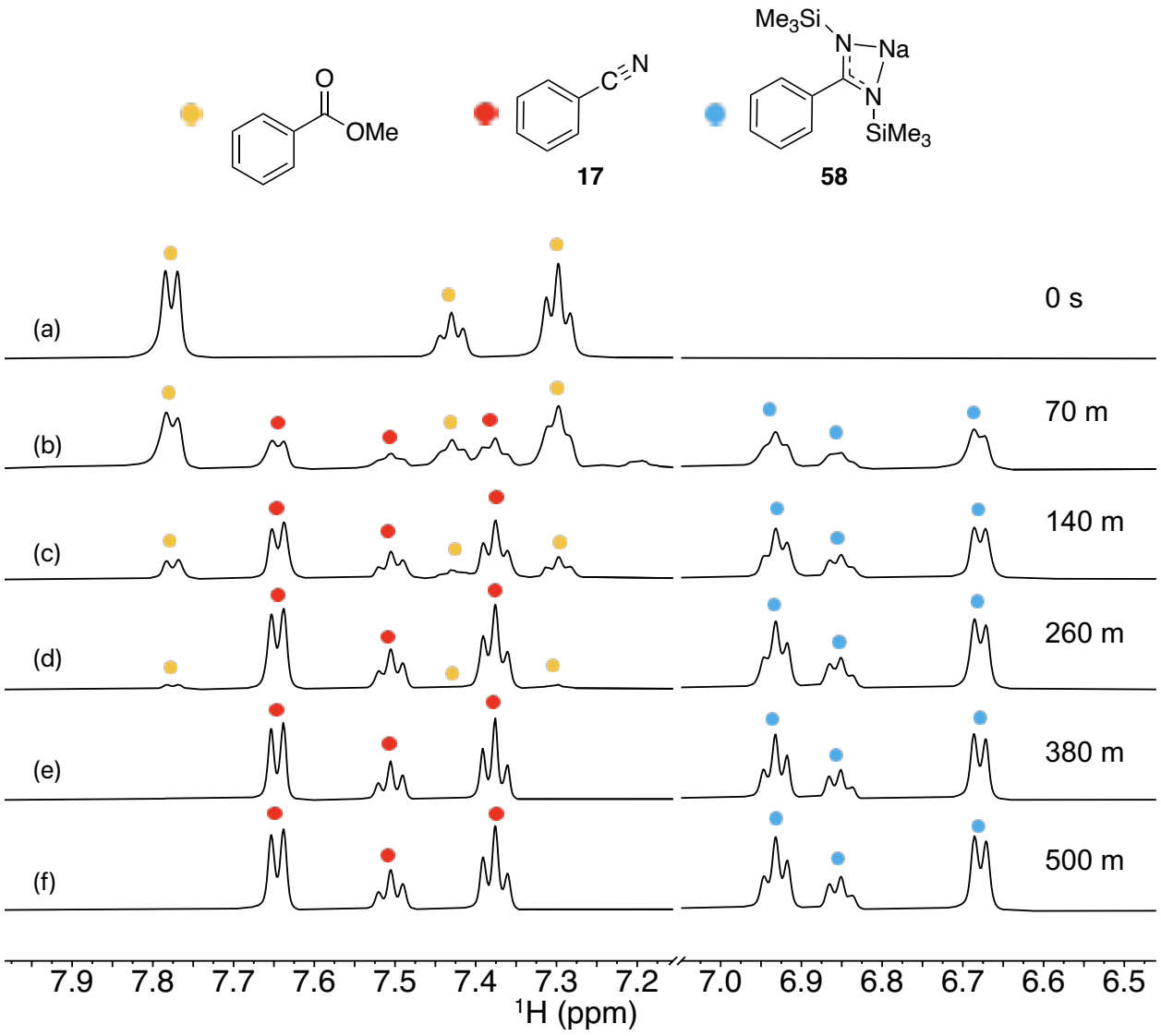
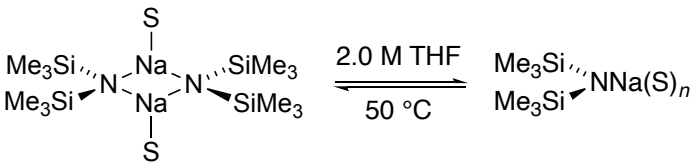
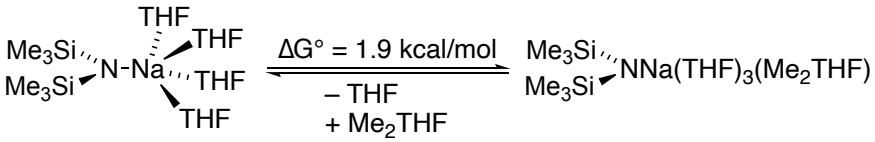


Figure S60. ^{1}H NMR spectra of a reaction mixture containing 0.050 M methyl benzoate and 0.15 M [^{15}N]NaHMDS in THF reacting at 80 °C, observed at –110 °C. Reaction

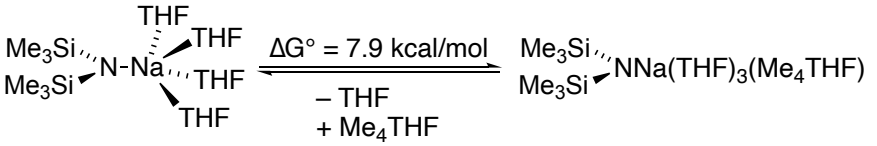
times for (a)–(f) are as follows: 0 m, 70 m, 140 m, 260 m, 380 m and 500 m respectively. Orange (●) represents methyl benzoate. Red (●) represents benzonitrile **17**. Blue (●) represents amidine **58**. ^{1}H spectra are referenced to a TMS internal standard (0.00 ppm).



cosolvent	monomer/ dimer
pentane	1 : 23
Me_2THF	1.3 : 1
Me_4THF	1 : 3



53 **53a**



53 **53b**

Figure S61. NaHMDS monomer/dimer ratio in THF/cosolvent mixture of choice pentane, 2,5-Me_2THF, 2,2,5,5-Me_4THF at 50 °C and DFT-computed solvation effect of 2,5-Me_2THF and 2,2,5,5-Me_4THF.

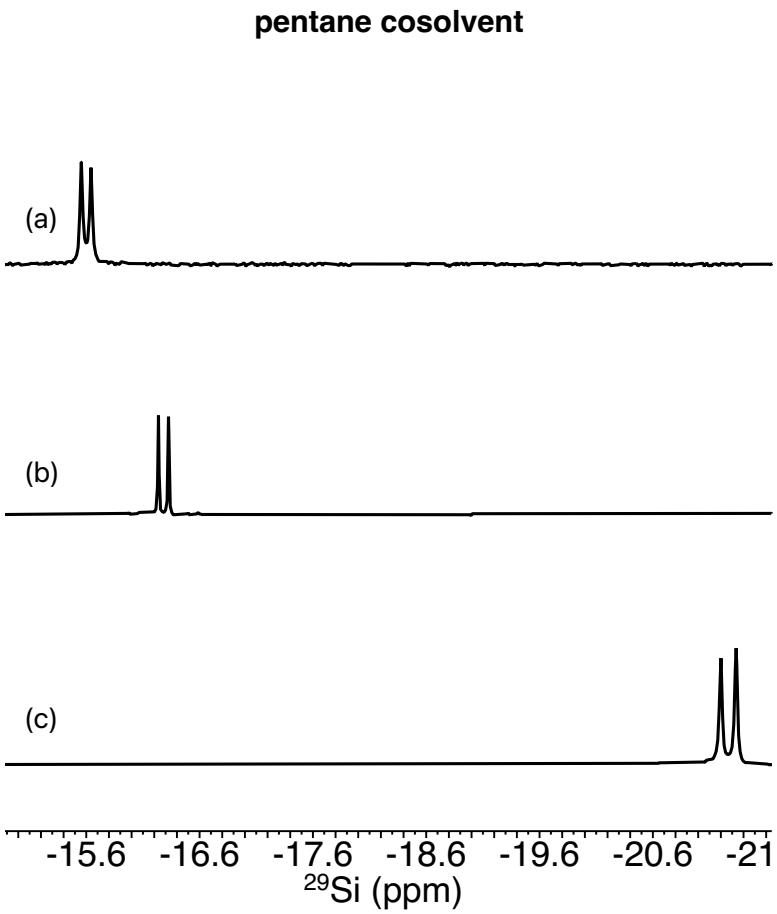


Figure S62. ^{29}Si NMR spectra of 0.10 M [^{15}N]NaHMDS in pentane varying the concentration of THF at 50 °C. THF concentration for (a)–(c) are as follows: 0.41, 2.00, and 12.31 M (neat), respectively. ^{29}Si spectra are referenced to a TMS internal standard (0.00 ppm). Concentrations for THF and coupling constants of the [^{15}N]NaHMDS ^{29}Si peaks are listed below.

[THF] (M) (pentane cosolvent)	**$^{1}J_{N–Si}$ coupling constant (Hz)**
0.41	8.62
2.00	8.81
12.31 (neat)	13.03

2,5-Me$_2$THF cosolvent

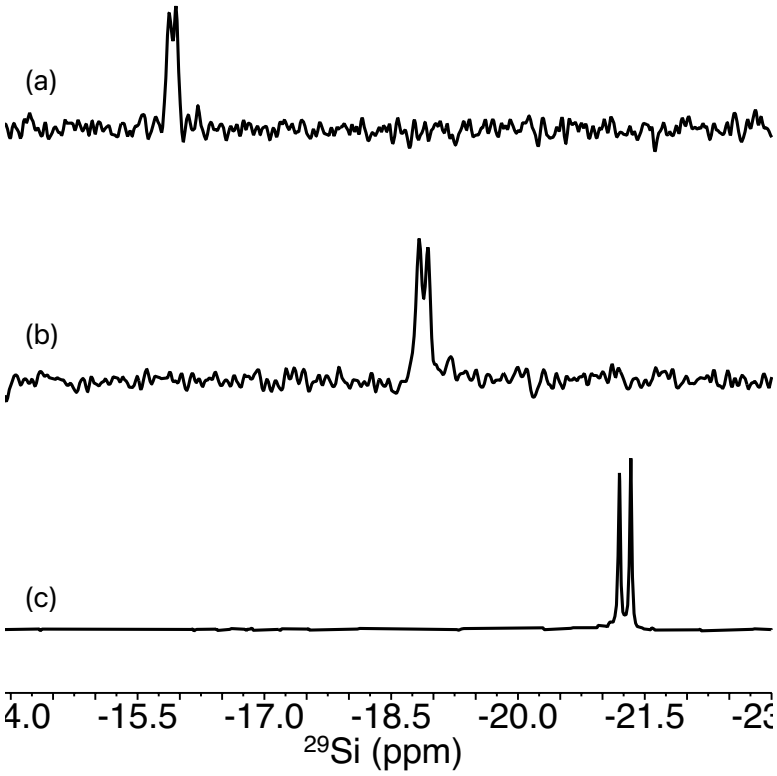


Figure S63. ^{29}Si NMR spectra of 0.10 M [^{15}N]NaHMDS in 2,5-Me$_2$THF varying the concentration of THF at 50 °C. THF concentration for (a)–(c) are as follows: 0.00, 2.00, and 12.31 M (neat), respectively. ^{29}Si spectra are referenced to a TMS internal standard (0.00 ppm). Concentrations for THF and coupling constants of the [^{15}N]NaHMDS ^{29}Si peaks are listed below.

[THF] (M) (2,5-dimethylTHF cosolvent)	**$^1J_{N–Si}$ coupling constant (Hz)**
0.00	8.81
2.00	11.23
12.31 (neat)	13.03

2,2,5,5-Me$_4$THF cosolvent

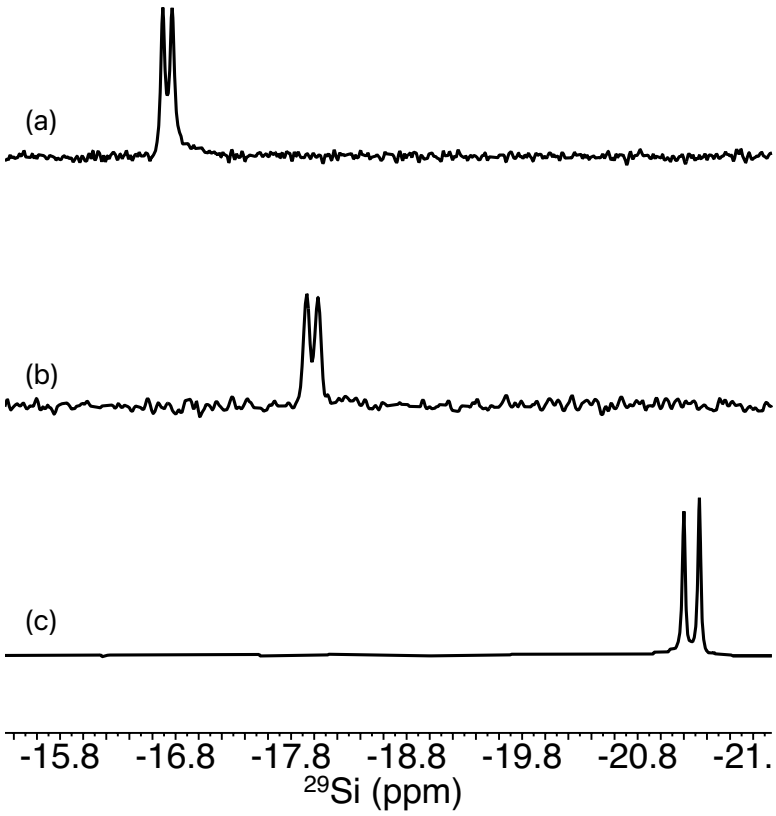


Figure S64. ^{29}Si NMR spectra of 0.10 M [^{15}N]NaHMDS in 2,2,5,5-Me$_4$THF varying the concentration of THF at 50 °C. THF concentration for (a)–(c) are as follows: 0.00, 2.00, and 12.31 M (neat), respectively. ^{29}Si spectra are referenced to a TMS internal standard (0.00 ppm). Concentrations for THF and coupling constants of the [^{15}N]NaHMDS ^{29}Si peaks are listed below.

[THF] (M) (2,2,5,5-tetramethylTHF cosolvent)	**$^1J_{N–Si}$ coupling constant (Hz)**
0.00	8.02
2.00	9.23
12.31 (neat)	13.03

Rate Studies

General procedure for in situ IR analyses

IR spectra were recorded with an in situ IR spectrometer fitted with a 30-bounce, silicon-tipped probe. The spectra were acquired at a gain of 1 and a resolution of 4 cm^{-1}. All tracked reactions were conducted under positive flow of argon from a Schlenk line.

A representative reaction was carried out as follows: The IR probe was inserted through a teflon adapter and O-ring seal into an oven-dried, cylindrical flask fitted with a magnetic stir bar and a T-joint. The T-joint was capped with a septum for injections and an argon line. After evacuation under full vacuum, heating, and flushing with argon, the flask was charged with the 0.1 M NaHMDS in THF/cosolvent mixture of choice 2,2,5,5-Me_4THF, 2,5-Me_2THF, pentane and cooled to 0 °C in the ice bath chiller and left to stir for 15 min.

A set of 256 baseline scans were collected and IR spectra were recorded every 15 seconds from 30 scans. At this point spectral collection was halted and an additional 256 baseline scans were collected. The spectrometer was configured to collect spectra ever 5 seconds from 16 scans. 1 set of scans was collected before addition of 0.12 M methyl picolinate in THF through the septum. The reaction was tracked over the disappearance of methyl picolinate complex (1733 cm^{-1}) and appearance of the imino-ether (1706 cm^{-1}).

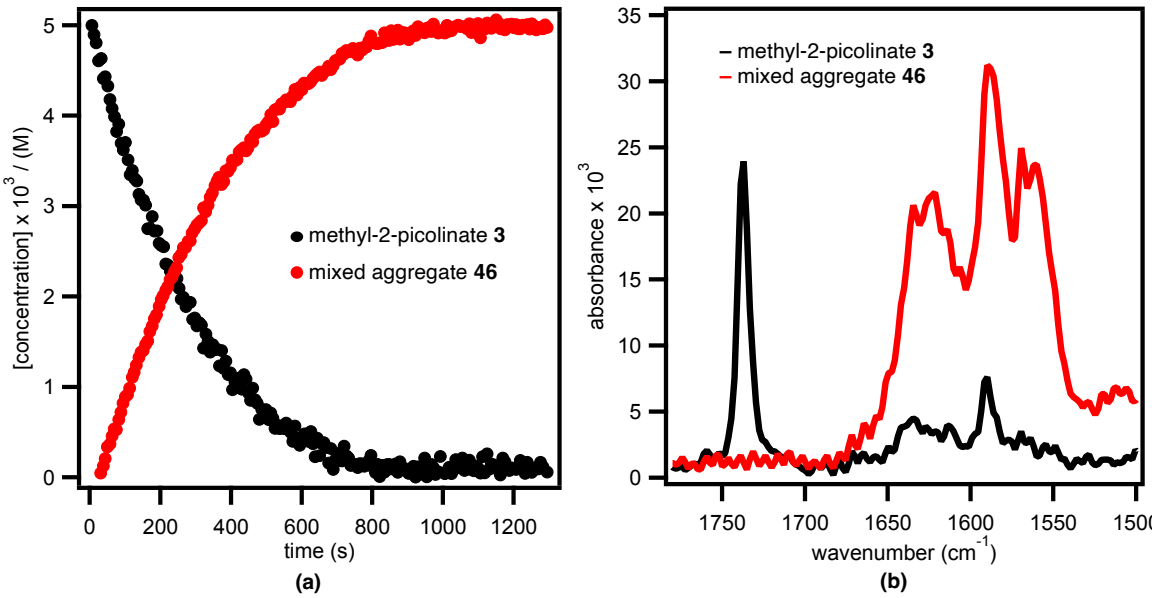


Figure S65. Emblematic addition of NaHMDS (0.10 M) to methyl-2-picolinate (**3**, 0.0050 M; 1737 cm^{-1}) to form mixed aggregate **46** (1584 cm^{-1}) at 25 °C in DMEA. (a) Plot of [methyl-2-picolinate **3**] (M) and [mixed aggregate **46**] (M) vs time (s). (b) IR spectra of methyl-2-picolinate **3** (first recorded spectrum) and mixed aggregate **46** (last recorded spectrum).

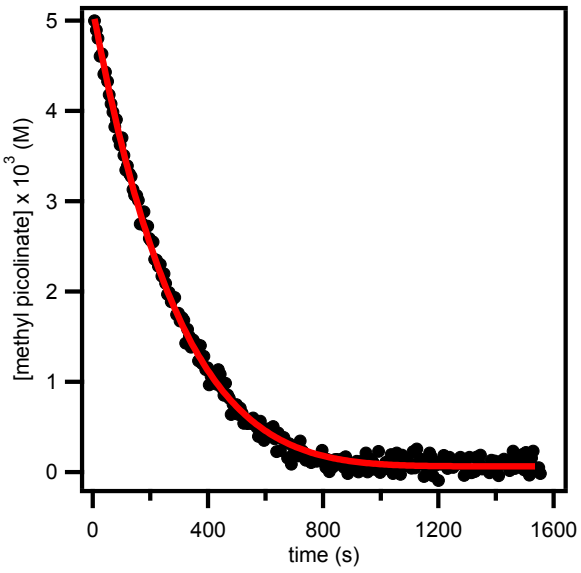


Figure S66. Addition of 0.0050 M NaHMDS to methyl-2-picolinate (**3**, 0.10 M) at 25 °C monitored by IR spectroscopy (1737 cm^{-1}). The curve depicts an unweighted least-squares fit to $y = ae^{-bx}$ ($a = 8.1 \times 10^{-3} \pm 0.1 \times 10^{-3}$; $b = 1.5 \times 10^{-3} \pm 0.1 \times 10^{-3}$).

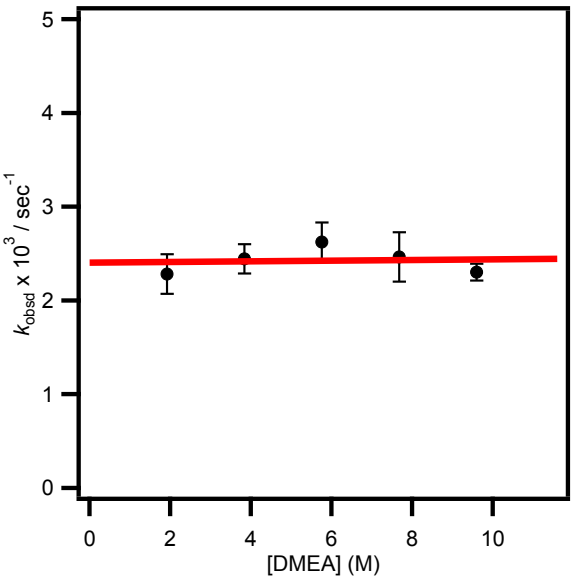


Figure S67. Plot of k_{obsd} vs [DMEA] (M) in pentane for the addition of NaHMDS (0.10 M) to methyl-2-picolinate (**3**, 0.0050 M) at 25 °C monitored by IR spectroscopy (1737 cm^{-1}). The curve depicts an unweighted least-squares fit to y = *a*x + *b* (*a* = 2.4 x 10^{-3} ± 0.2 x 10^{-4}; *b* = 3.3 x 10^{-6} ± 0.3 x 10^{-6}).

Table S1. Average pseudo-first-order rate constants (k_{obsd}) at various DMEA (pentane cosolvent) concentrations for the addition of NaHMDS (0.10 M) to methyl-2-picolinate (**3**, 0.0050 M) at 25 °C.

[DMEA] / M	k_{obsd} x 10^3 / sec^{-1}	Standard Deviation x 10^3/ sec^{-1}
1.92	2.28	0.21
3.84	2.60	0.16
5.76	2.83	0.21
7.68	2.72	0.26
9.60 (neat)	2.39	0.09

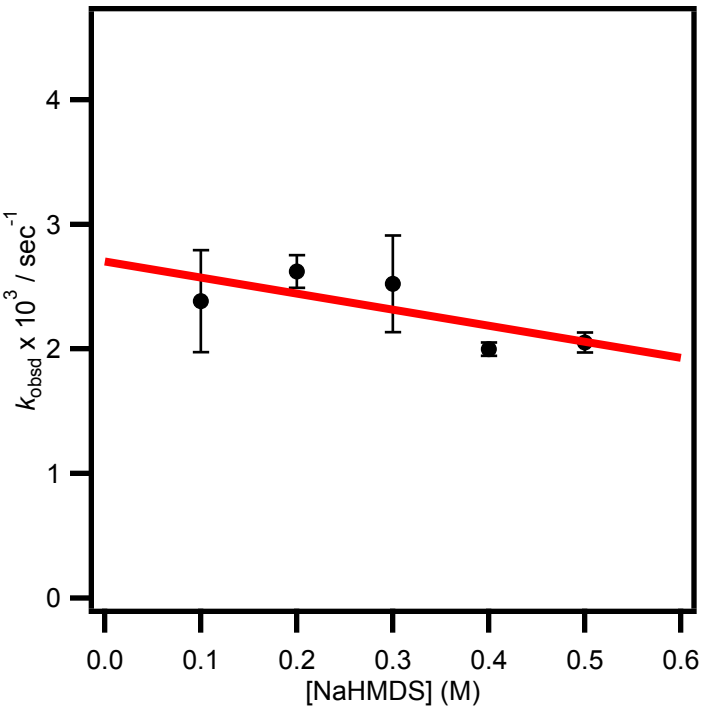


Figure S68. Plot of k_{obsd} vs [NaHMDS] (M) for the addition of NaHMDS to methyl-2-picolinate (**3**, 0.050 M) in 9.6 M (neat) DMEA at 25 °C monitored by IR spectroscopy (1737 cm^{-1}). The curve depicts an unweighted least-squares fit to y = *a*x + *b* (*a* = 2.7 x 10^{-3} ± 0.2 x 10^{-3}; *b* = –1.3 x 10^{-3} ± 0.1 x 10^{-3}).

Table S2. Average pseudo-first-order rate constants (k_{obsd}) at various NaHMDS concentrations for the addition of NaHMDS to methyl-2-picolinate (**3**, 0.0050 M) in 9.60 M (neat) DMEA at 25 °C.

[NaHMDS] / M	k_{obsd} x 10^3 / sec^{-1}	Standard Deviation x 10^3/ sec^{-1}
0.1	2.38	0.41
0.2	2.62	0.13
0.3	2.52	0.38
0.4	1.99	0.05
0.5	2.05	0.08

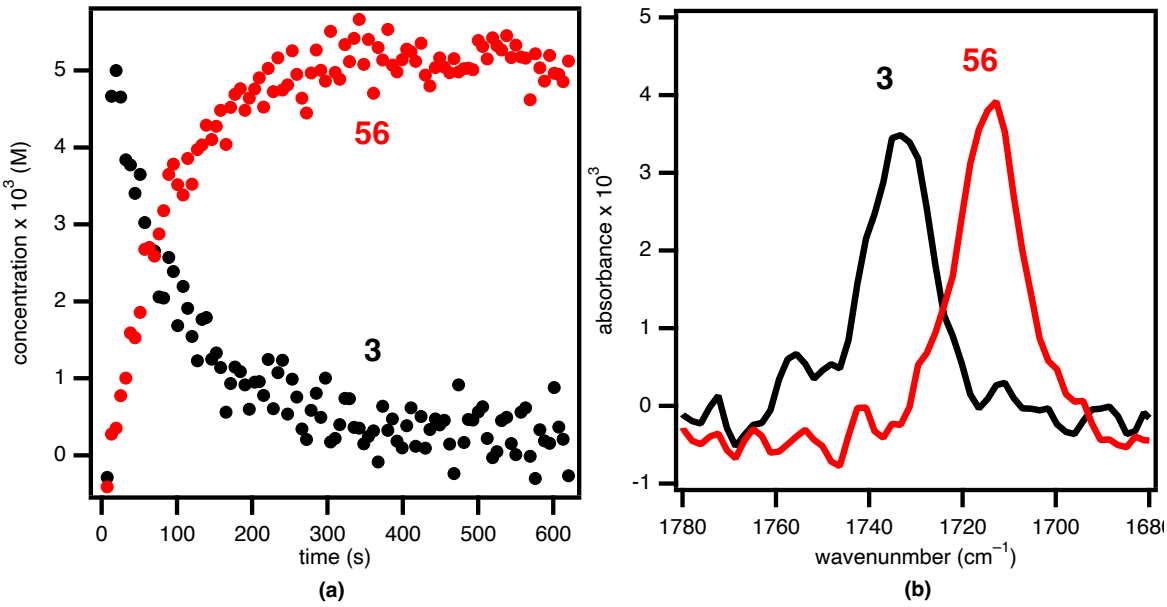


Figure S69. Emblematic addition of NaHMDS (0.10 M) to methyl-2-picolinate (**3**, 0.0050 M; 1734 cm^{-1}) to form imino ether **56** (1713 cm^{-1}) at 25 °C in DMEA. (a) Plot of [methyl-2-picolinate **3**] (M) and [imino ether **56**] (M) vs time (s). (b) IR spectra of methyl-2-picolinate **3** (first recorded spectrum) and imino ether **56** (last recorded spectrum).

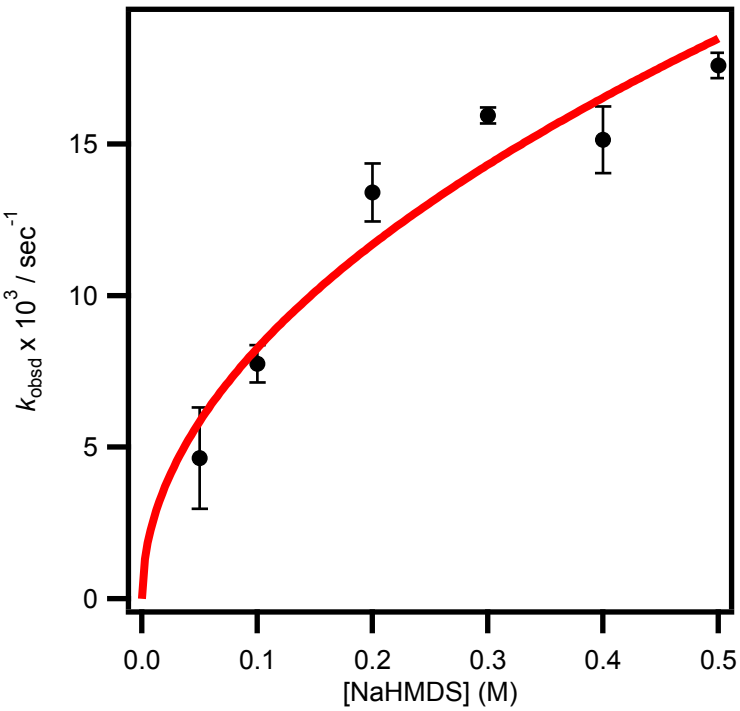


Figure S70. Plot of k_{obsd} vs [NaHMDS] (M) for the addition of NaHMDS to methyl-2-picolinate (**3**, 0.0050 M) in 12.8 M (neat) THF at 0 °C monitored by IR spectroscopy (1731 cm^{-1}). The curve depicts an unweighted least-squares fit to $y = ax^n$ ($a = 2.4 \times 10^{-3} \pm 0.1 \times 10^{-3}$; $n = 0.44 \pm 0.01$).

Table S3. Average pseudo-first-order rate constants (k_{obsd}) at various NaHMDS concentrations for for the addition of NaHMDS to methyl-2-picolinate (**3**, 0.0050 M) in 12.8 M (neat) THF at 0 °C.

[NaHMDS] / M	k_{obsd} x 10^3 / sec^{-1}	Standard Deviation x 10^3/ sec^{-1}
0.05	4.64	0.61
0.1	7.75	0.95
0.2	13.40	2.62
0.3	15.94	1.11
0.4	15.14	0.42
0.5	17.59	1.67

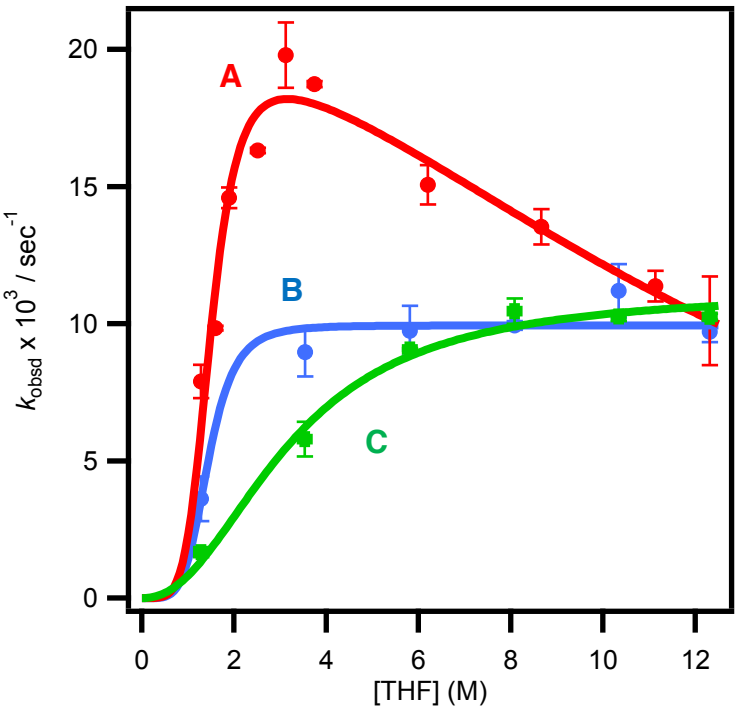


Figure S71. Plot of k_{obsd} vs [THF] (M) for the addition of NaHMDS to methyl-2-picolinate (**3**, 0.0050 M) in 0.10 M NaHMDS at 0 °C monitored by IR spectroscopy (1732 cm^{-1}). Curve A (Red) derives from pentane cosolvent and depicts an unweighted least-squares fit to $ax^n/(1+ bx^n)(1/1+cx^2)$ ($a = 2.4 \times 10^{-3} \pm 0.1 \times 10^{-3}$; $b = 1.3 \times 10^{-1} \pm 0.1 \times 10^{-1}$; $c = 0.6 \times 10^{-3} \pm 0.1 \times 10^{-4}$; $n = 5$). Curve B (Blue) derives from 2,5-Me_2THF cosolvent and depicts an unweighted least-squares fit to $y = ax^n/(1+ bx^n)$ ($a = 1.6 \times 10^{-1} \pm 0.1 \times 10^{-1}$; $b = 1.6 \times 10^{-1} \pm 0.1 \times 10^{-1}$; $n = 5$). Curve C (Green) derives from 2,2,5,5-Me_4THF cosolvent and depicts an unweighted least-squares fit to $y = ax^n/(1+ bx^n)$ ($a = 8.2 \times 10^{-4} \pm 0.1 \times 10^{-1}$; $b = 7.9 \times 10^{-2} \pm 0.1 \times 10^{-2}$; $n = 2.2 \pm 0.2$).

Table S4. Average pseudo-first-order rate constants (k_{obsd}) at various THF (pentane cosolvent) concentrations for the addition of NaHMDS (0.10 M) to methyl-2-picolinate (**3**, 0.0050 M) at 0 °C.

Red

Cosolvent:	pentane	
[THF] / M	k_{obsd} x 10^3 / sec^{-1}	Standard Deviation x 10^3 / sec^{-1}
1.28	7.90	0.61
1.59	9.83	0.09
1.89	14.59	0.37
2.51	16.32	0.10
3.12	19.79	1.18
3.74	18.74	0.11
6.2	15.06	0.71
8.66	13.53	0.64
11.13	11.37	0.56
12.31	10.11	1.61

Table S5. Average pseudo-first-order rate constants (k_{obsd}) at various THF (2,5-Me_2THF cosolvent) concentrations for the addition of NaHMDS (0.10 M) to methyl-2-picolinate (**3**, 0.0050 M) at 0 °C.

Blue

Cosolvent:	2,5-Me_2THF	
[THF] / M	k_{obsd} x 10^3 / sec^{-1}	Standard Deviation x 10^3 / sec^{-1}
1.28	3.62	0.81
3.54	8.96	0.89
5.81	9.74	0.90
8.08	9.93	0.15
10.34	11.20	0.97
12.31	9.71	0.37

Table S6. Average pseudo-first-order rate constants (k_{obsd}) at various THF (2,2,5,5-Me_4THF cosolvent) concentrations for the addition of NaHMDS (0.10 M) to methyl-2-picolinate (**3**, 0.0050 M) at 0 °C.

Green

Cosolvent:	2,2,5,5-Me_4THF	
[THF] / M	k_{obsd} x 10^3 / sec^{-1}	Standard Deviation x 10^3 / sec^{-1}
1.28	1.67	0.18
3.54	5.79	0.63
5.81	9.06	0.05
8.08	10.46	0.46
10.34	10.26	0.18
12.31	10.25	0.11

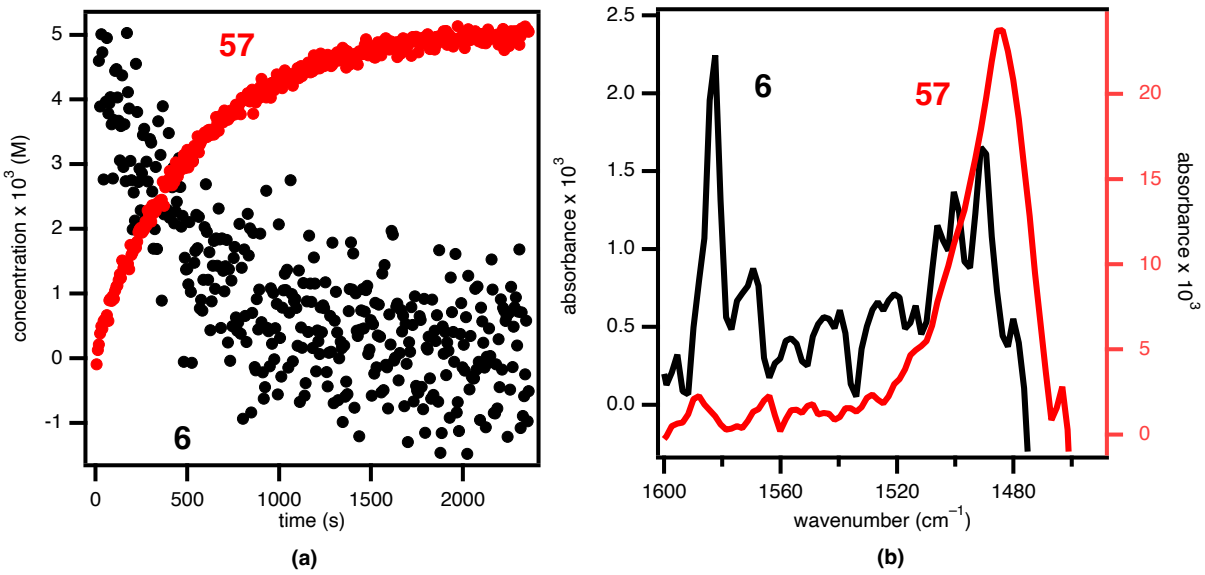


Figure S72. Emblematic addition of NaHMDS (0.10 M) to picolinonitrile (**6**, 0.0050 M; 1584 cm^{-1}) to form silyated amidine **57** (1486 cm^{-1}) at –20 °C in THF. (a) Plot of [picolinonitrile **6**] (M) and [silyated amidine **57**] (M) vs time (s). (b) IR spectra of picolinonitrile **6** (first recorded spectrum) and silyated amidine **57** (last recorded spectrum).

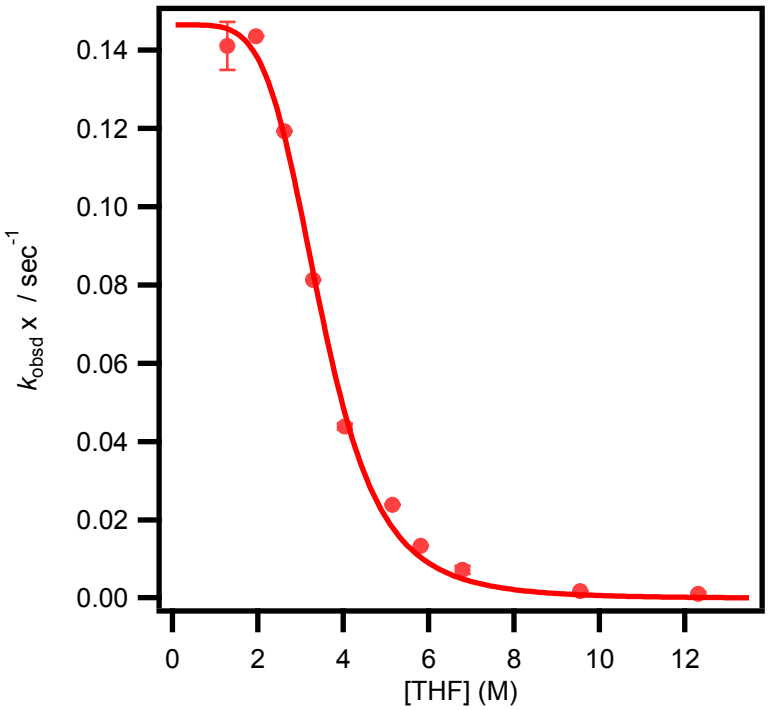


Figure S73. Plot of k_{obsd} vs [THF] (M) for the addition of NaHMDS to picolinonitrile (**6**, 0.0050 M) in 0.10 M NaHMDS at –20 °C monitored by IR spectroscopy (1584 cm^{-1}). Curve A (red) derives from pentane cosolvent and depicts an unweighted least-squares fit to $ax^n/(1 + bx^n)$ ($a = 2.5 \times 10^1 \pm 0.5 \times 10^{-1}$; $b = 1.7 \times 10^2 \pm 0.8 \times 10^{-2}$; $n = -5.8 \pm 0.2$).

Table S7. Average pseudo-first-order rate constants (k_{obsd}) at various THF (pentane cosolvent) concentrations for the addition of NaHMDS (0.10 M) to picolinonitrile (**6**, 0.0050 M) at –20 °C.

Cosolvent:	pentane	
[THF] / M	k_{obsd} / sec^{-1}	Standard Deviation / sec^{-1}
1.28	0.141	0.006
1.95	0.143	*not replicated*
2.62	0.119	*not replicated*
3.29	0.0813	*not replicated*
4.03	0.0439	0.0008
5.15	0.0239	*not replicated*
5.81	0.0134	*not replicated*
6.79	0.00730	0.001
9.55	0.00188	0.0007
12.31	0.00119	0.0004

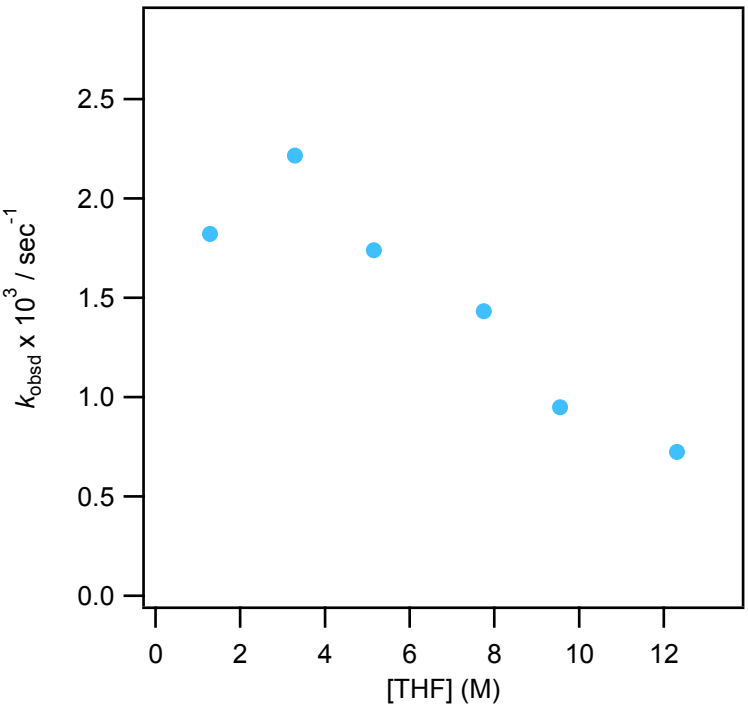


Figure S74. Plot of k_{obsd} vs [THF] (M) for the addition of NaHMDS to picolinonitrile (**6**, 0.0050 M) in 0.10 M NaHMDS at –20 °C monitored by IR spectroscopy (1584 cm^{-1}), utilizing 2,5-Me_2THF as cosolvent.

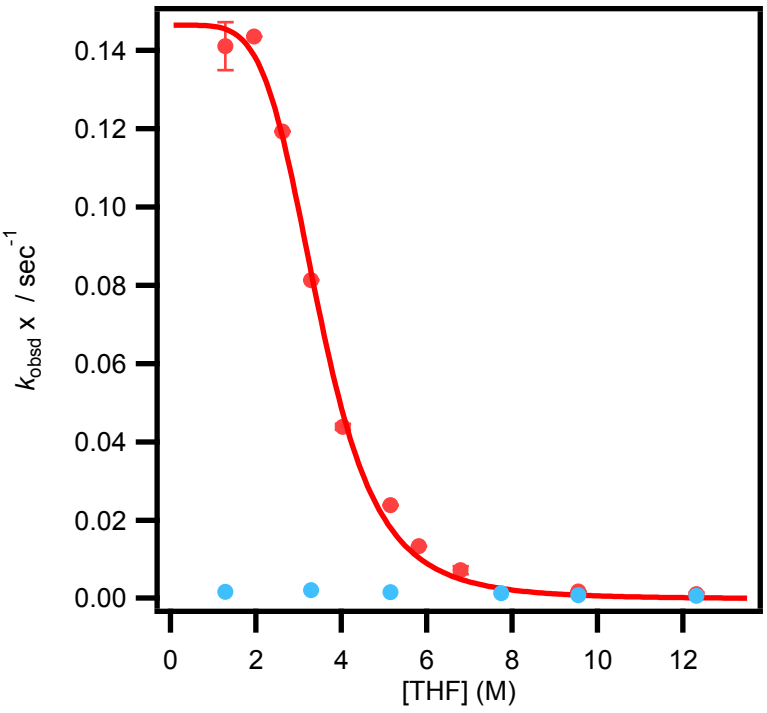


Figure S75. Plot of k_{obsd} vs [THF] (M) for the addition of NaHMDS to picolinonitrile (**6**, 0.0050 M) in 0.10 M NaHMDS at –20 °C monitored by IR spectroscopy (1584 cm^{-1}). Curve A (red) derives from pentane cosolvent. Curve B (blue) derives from 2,5-Me$_2$THF cosolvent. The large rate difference between the two curves might be attributed to the difference in the NaHMDS ground state monomer/dimer ratio of the pentane cosolvent and 2,5-Me$_2$THF cosolvent at low THF concentration.

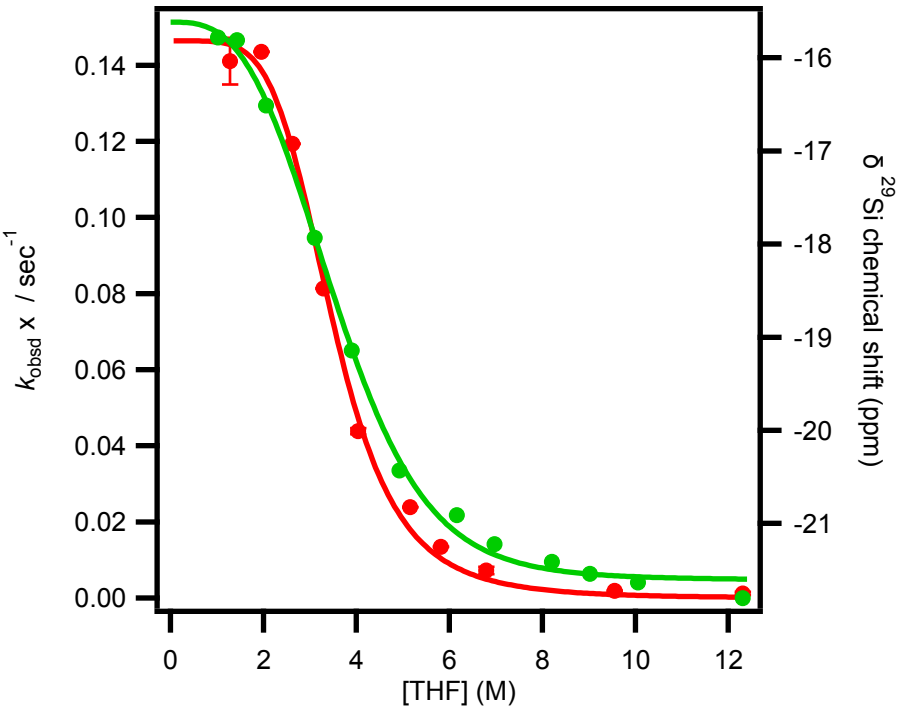


Figure S76. Plot of k_{obsd} vs [THF] (M) for the addition of NaHMDS to picolinonitrile (**6**) in pentane cosovent (red) and ^{29}Si chemical shift (green) plotted versus [THF] in 2:1 pentane/toluene as cosolvent measured at –20 °C. The latter plot fits to a model based on an A_2S_2–AS_4 equilibrium.

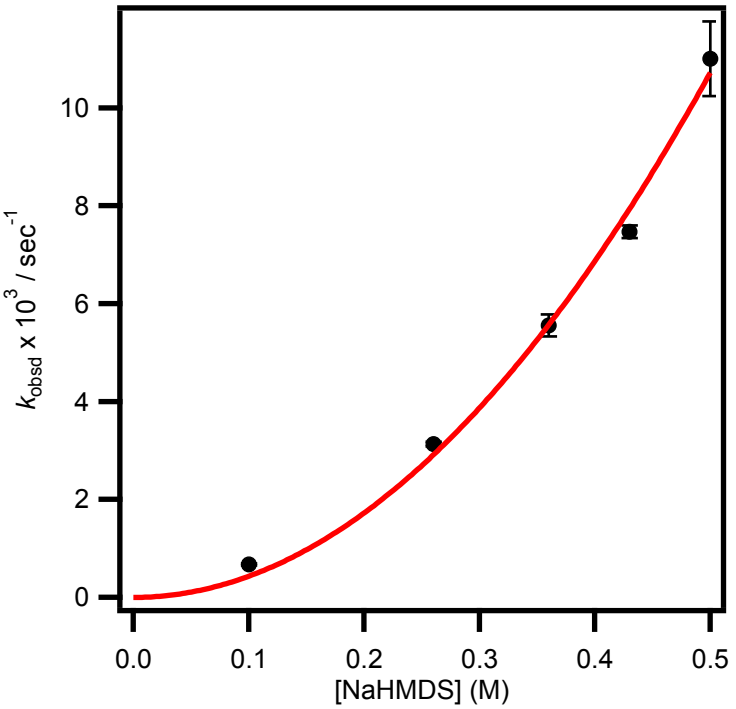


Figure S77. Plot of k_{obsd} vs [NaHMDS] (M) for the addition of NaHMDS to picolinonitrile (**6**, 0.0050 M) in 12.8 M (neat) THF at –20 °C monitored by IR spectroscopy (1584 cm^{-1}). The curve depicts an unweighted least-squares fit to $y = ax^n$ ($a = 4.3 \times 10^{-2} \pm 0.1 \times 10^{-2}$; $n = 2.0 \pm 0.1$).

Table S8. Average pseudo-first-order rate constants (k_{obsd}) at various NaHMDS concentrations for the addition of NaHMDS to picolinonitrile (**6**, 0.0050 M) in 9.6 M (neat) DMEA at 25 °C.

[NaHMDS] / M	k_{obsd} x 10^3 / sec^{-1}	Standard Deviation x 10^3/ sec^{-1}
0.1	0.67	0.02
0.2	3.13	0.05
0.3	5.78	0.22
0.4	7.56	0.13
0.5	11.77	0.76

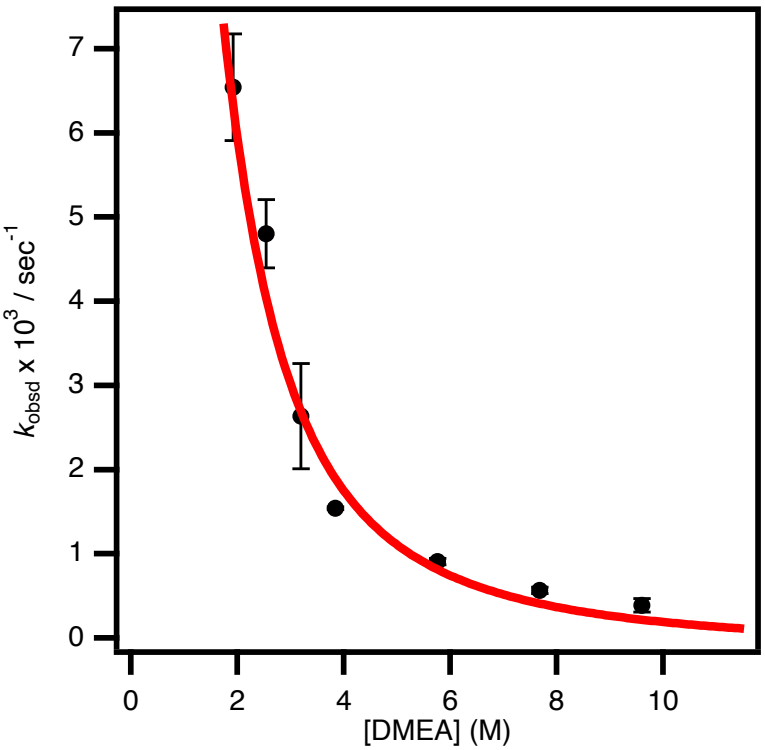


Figure S78. Plot of k_{obsd} vs [DMEA] (M) in pentane for the addition of NaHMDS (0.10 M) to picolinonitrile (**6**, 0.0050 M) at –40 °C monitored by IR spectroscopy (1584 cm^{-1}). The curve depicts an unweighted least-squares fit to $y = ax^n/(1+bx^n)$ ($n = -1.9 \pm 0.1$; $a = 2.3 \times 10^{-2} \pm 0.1 \times 10^{-2}$; $b = 1.7 \times 10^{-1} \pm 0.1 \times 10^{-1}$).

Table S9. Average pseudo-first-order rate constants (k_{obsd}) at various DMEA (pentane cosolvent) concentrations for the addition of NaHMDS (0.10 M) to picolinonitrile (**6**, 0.0050 M) at –40 °C.

[DMEA] / M	k_{obsd} x 10^3 / sec^{-1}	Standard Deviation x 10^3/ sec^{-1}
1.92	6.54	0.63
2.54	4.80	0.41
3.19	2.63	0.02
3.84	1.54	0.04
5.76	0.91	0.04
7.68	0.57	0.04
9.60 (neat)	0.38	0.03

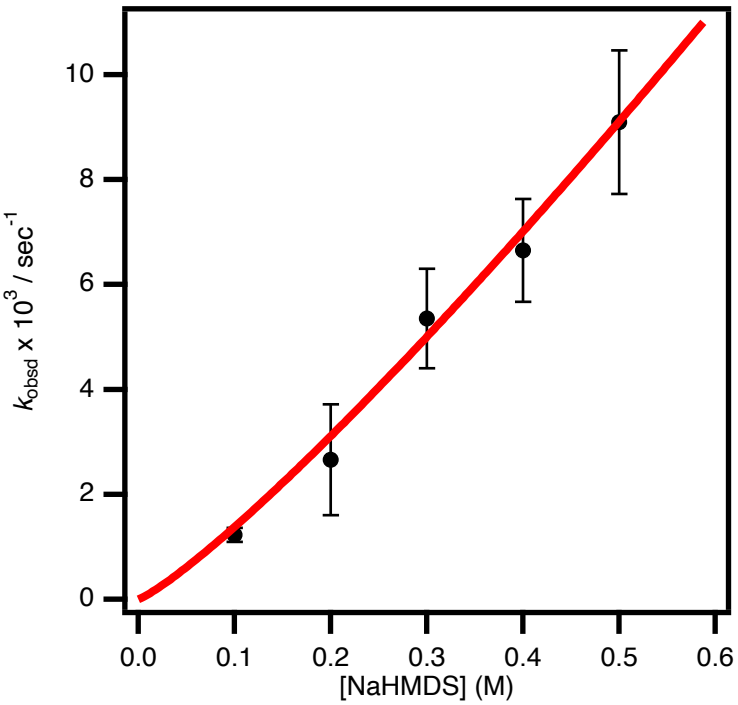


Figure S79. Plot of k_{obsd} vs [NaHMDS] (M) for the addition of NaHMDS to picolinonitrile (**6**, 0.0050 M) in 9.6 M (neat) DMEA at –40 °C monitored by IR spectroscopy (1584 cm^{-1}). The curve depicts an unweighted least-squares fit to $y = ax^n$ ($a = 2.1 \times 10^{-2} \pm 0.1 \times 10^{-2}$; $n = 1.1 \pm 0.1$).

Table S10. Average pseudo-first-order rate constants (k_{obsd}) at various NaHMDS concentrations for the addition of NaHMDS to picolinonitrile (**6**, 0.0050 M) in 9.6 M (neat) DMEA at –40 °C.

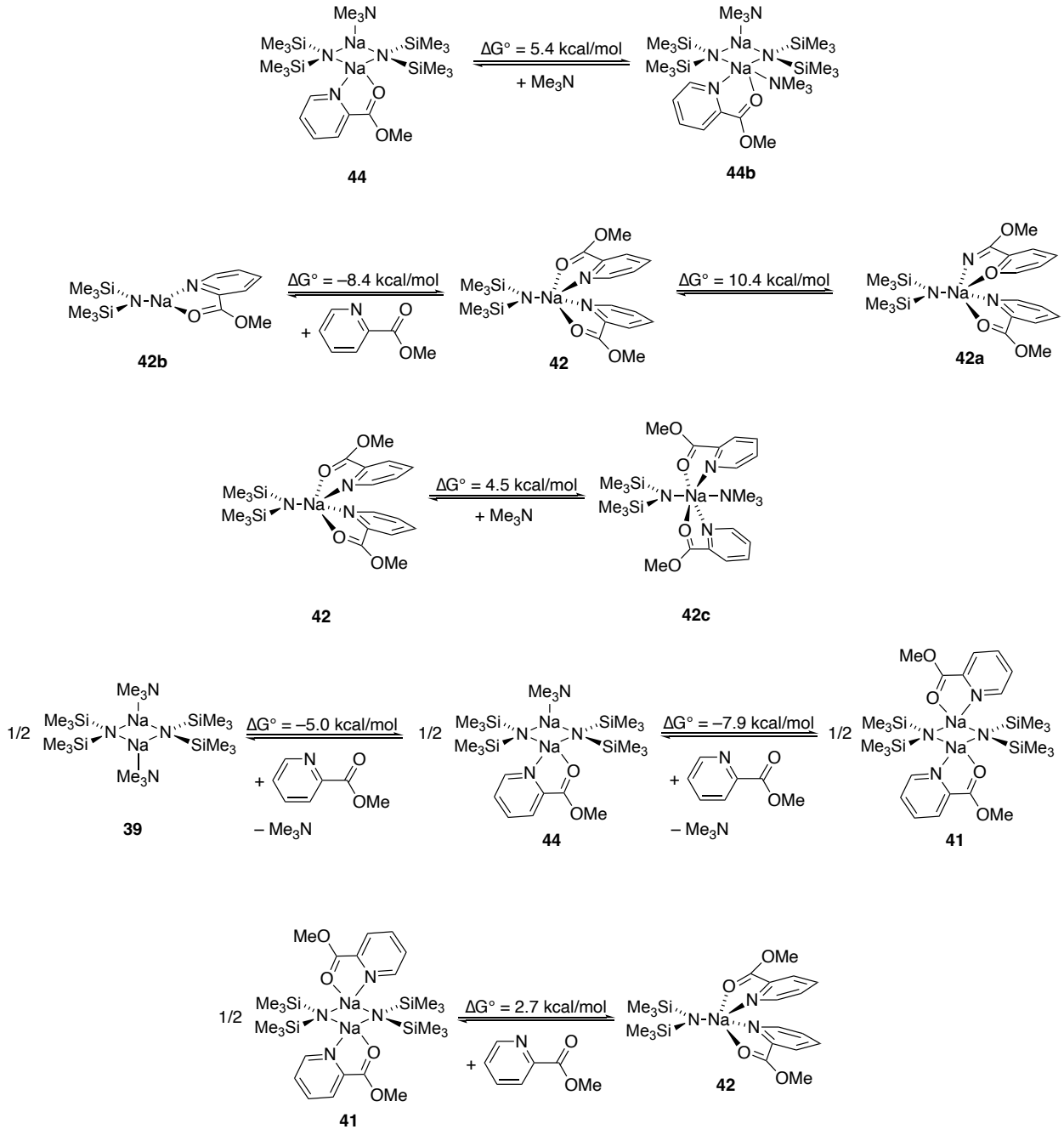
[NaHMDS] / M	k_{obsd} x 10^3 / sec^{-1}	Standard Deviation x 10^3/ sec^{-1}
0.1	1.23	0.13
0.2	2.66	1.05
0.3	5.35	0.94
0.4	6.65	0.98
0.5	9.09	1.36

Computational Data

General computational methods

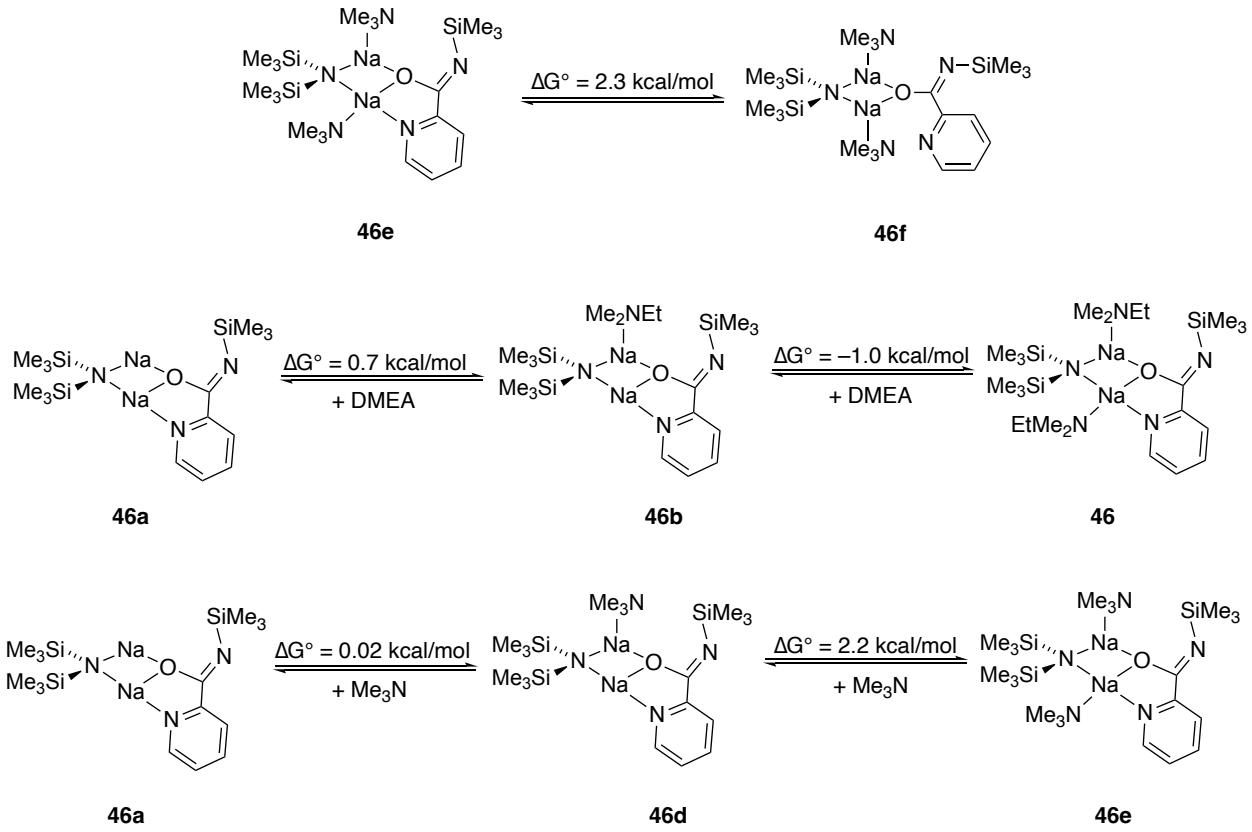
DFT calculations were performed with the Gaussian 16 program package. Geometry optimizations and single point energies were computed at the M06-2X/def2-SVP level of theory and M06-2X/def2-TZVP level of theory respectively. A pruned (99,590) integration grid was used for all computations as well. CYLview Visualization Software was used for all ball-and- stick structures. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the M06-2X level of theory (Hartrees; T = 298.15 K). G_{SP} is derived from a single point calculation corresponding to the DFT-optimized geometry with the larger basis set (def2-TZVP) and includes a thermal correction from the optimization. Hydrogens have been removed from ball-and-stick models to improve clarity. A vibrational frequency analysis was conducted at the same level of theory as the geometry optimizations (M06-2X/def2-SVP). The optimized geometries characterized as local minima on the potential energy surface have no imaginary frequencies, while each transition state possesses exactly one. Transition structures were verified with bi-directional IRC calculations.

DFT-computed ground state structures of methyl picolinate 3 and NaHMDS in DMEA



Scheme S1. DFT-computed free energies for the methyl picolinate **3** and NaHMDS complexed ground state structures in DMEA using Me_3N as a DMEA surrogate.

DFT-computed ground state structures of mixed aggregate 46



Scheme S2. DFT-computed free energies for the mixed aggregate **46** and serial solvation of mixed aggregate **46** with Me_3N.

Reaction coordinate aminolysis of methyl-2-picolinate (3) by NaHMDS in DMEA using Me_3N as a DMEA surrogate.

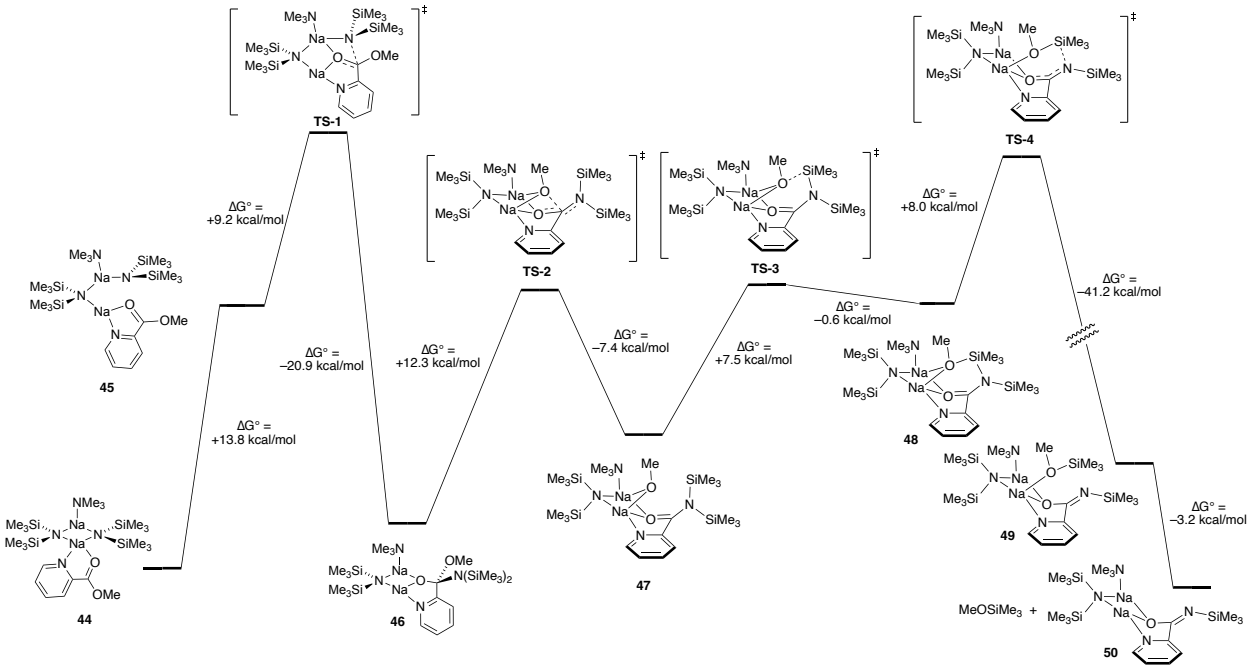


Figure S80. DFT-computed reaction coordinate aminolysis of methyl-2-picolinate (**3**) by NaHMDS in DMEA using Me_3N as a DMEA surrogate.

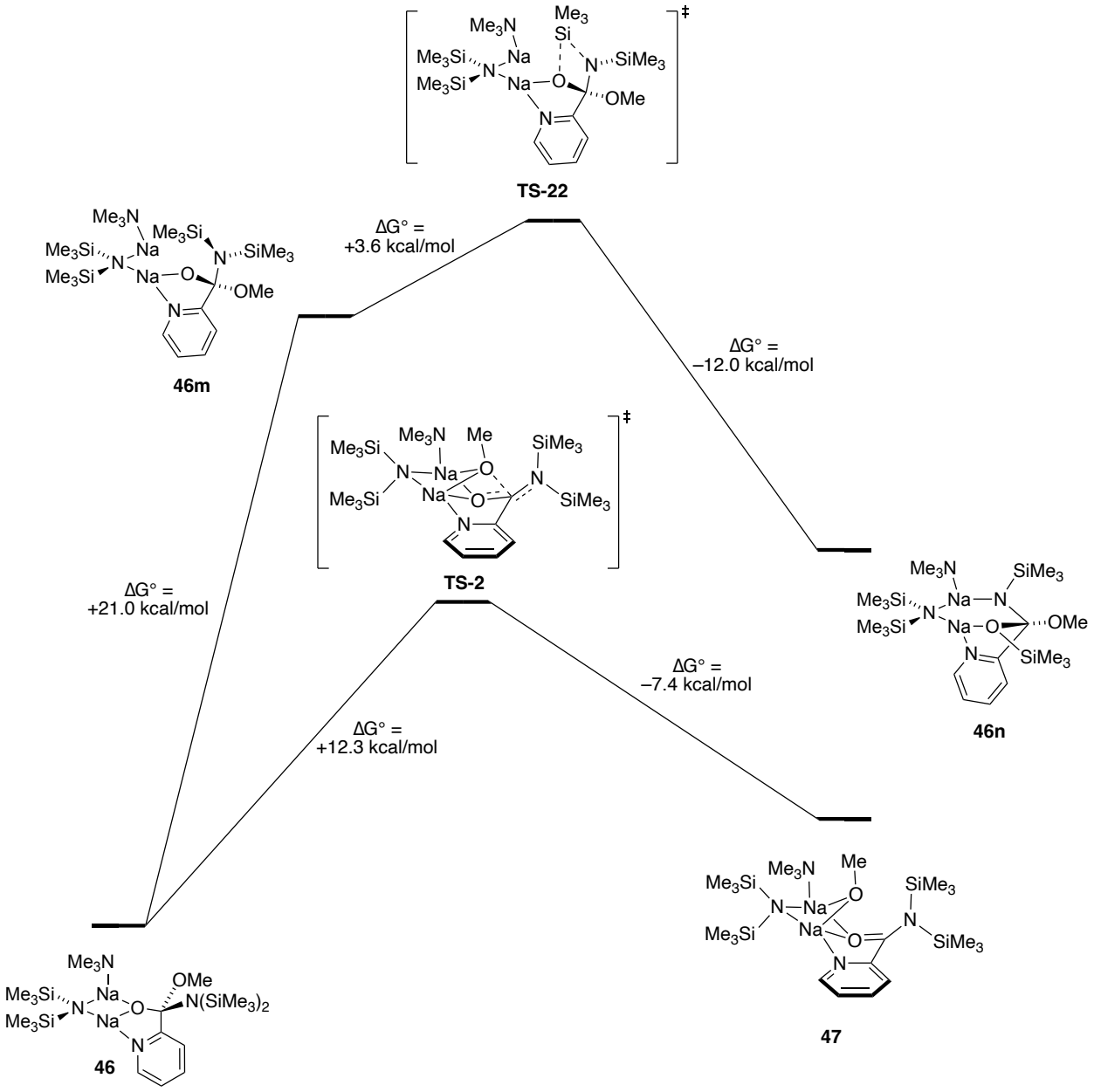
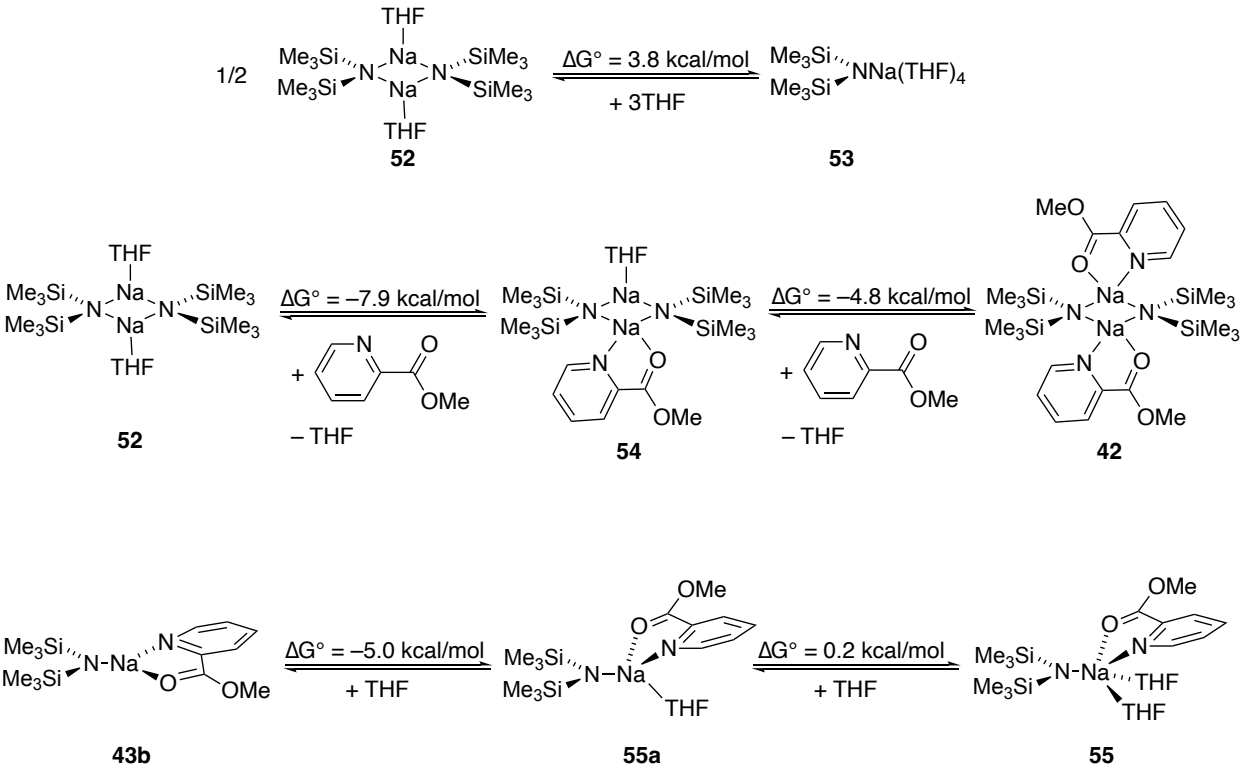


Figure S81. DFT-computed other pathway (carbonyl oxygen attacking TMS instead of methoxide group leaving) reaction coordinate aminolysis of methyl-2-picolinate (**3**) by NaHMDS using Me_3N as a DMEA surrogate, starting from **46**.

DFT-computed ground state structures of methyl picolinate 3 and NaHMDS in THF



Scheme S3. DFT-computed free energies for the methyl picolinate **3** and NaHMDS complexed ground state structures in THF.

Reaction coordinate aminolysis of methyl-2-picolinate (3) by NaHMDS in THF

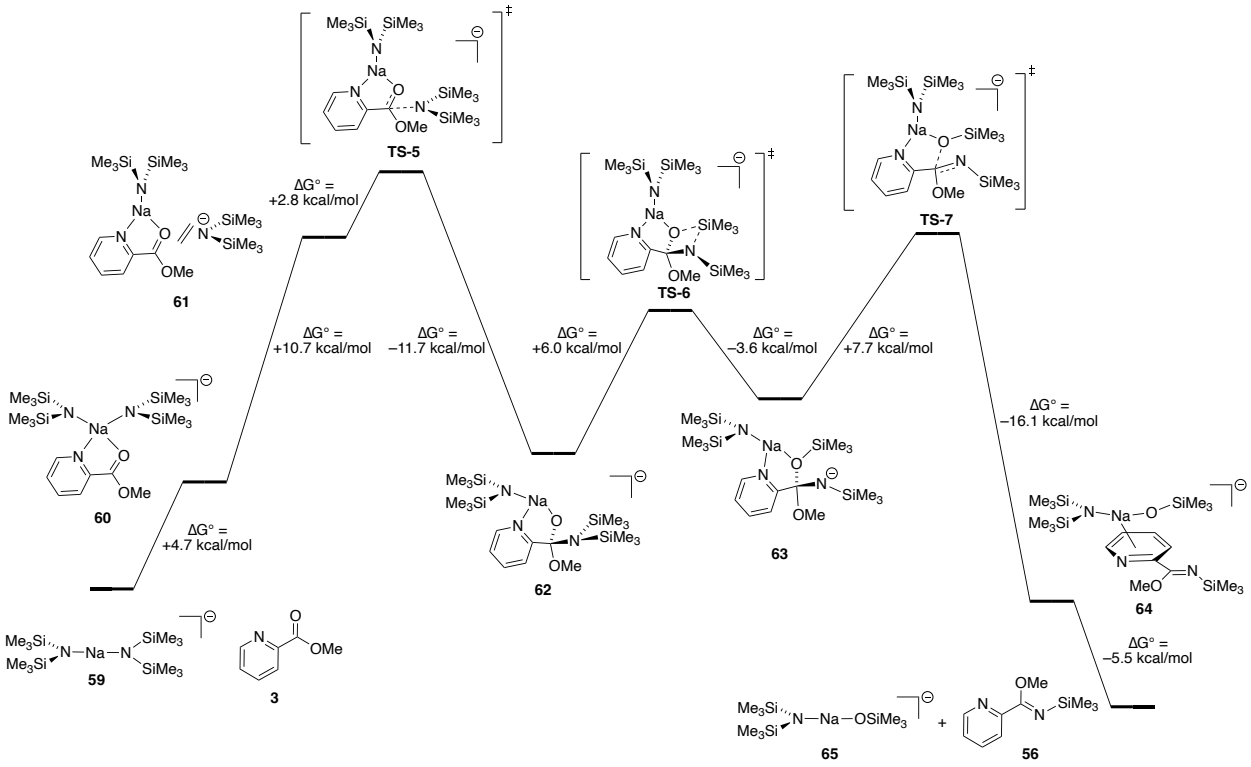


Figure S82. DFT-computed reaction coordinate aminolysis of methyl-2-picolinate (**3**) by NaHMDS in THF.

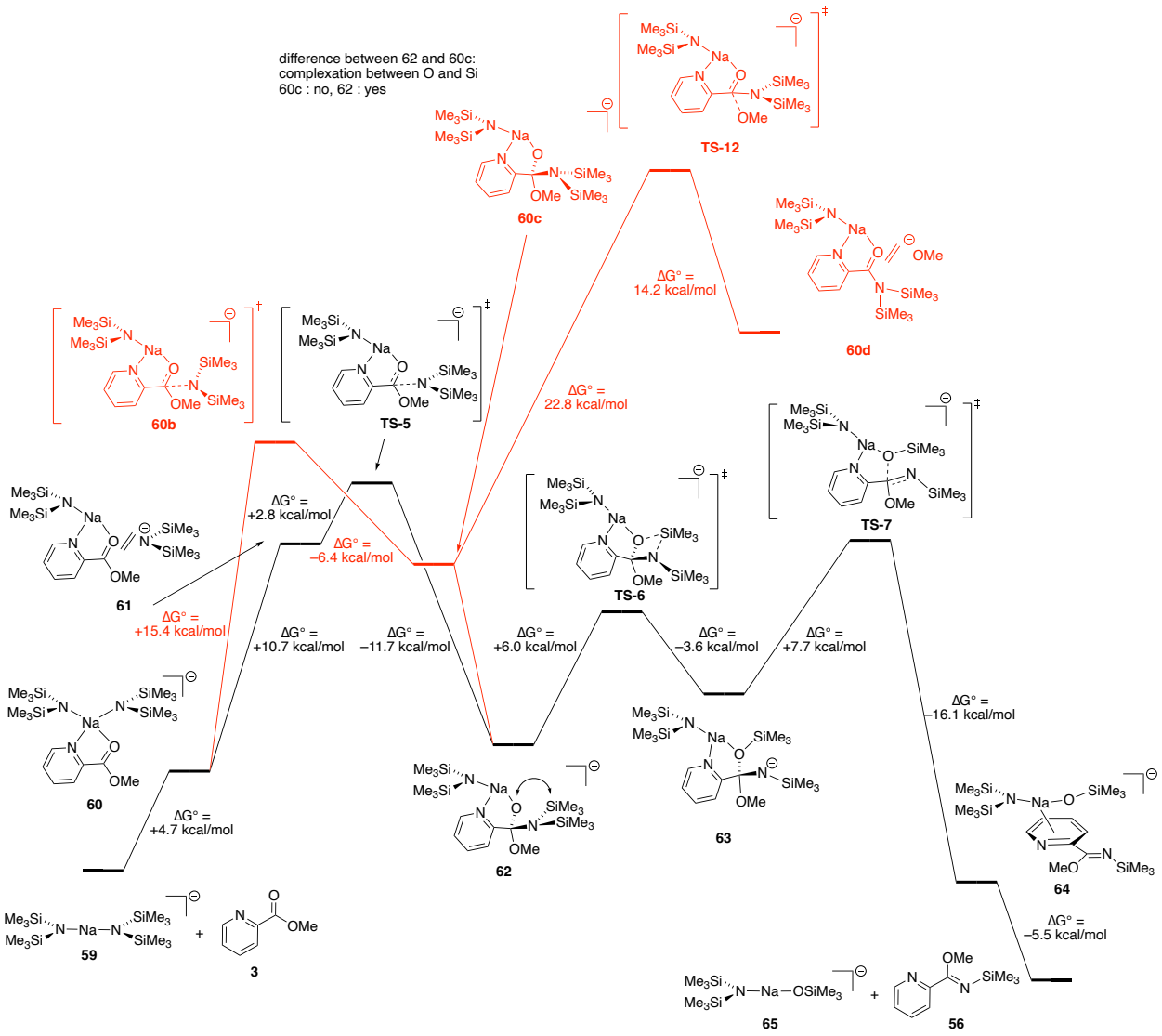


Figure S83. DFT-computed reaction coordinate aminolysis of methyl-2-picolinate (**3**) by NaHMDS in THF, containing an alternative pathway (methoxide group leaving instead of carbonyl oxygen attacking the TMS).

DFT-computed reaction coordinate of 1,2-addition by picolinonitrile (6) and NaHMDS, and subsequent amidine (56) formation in THF

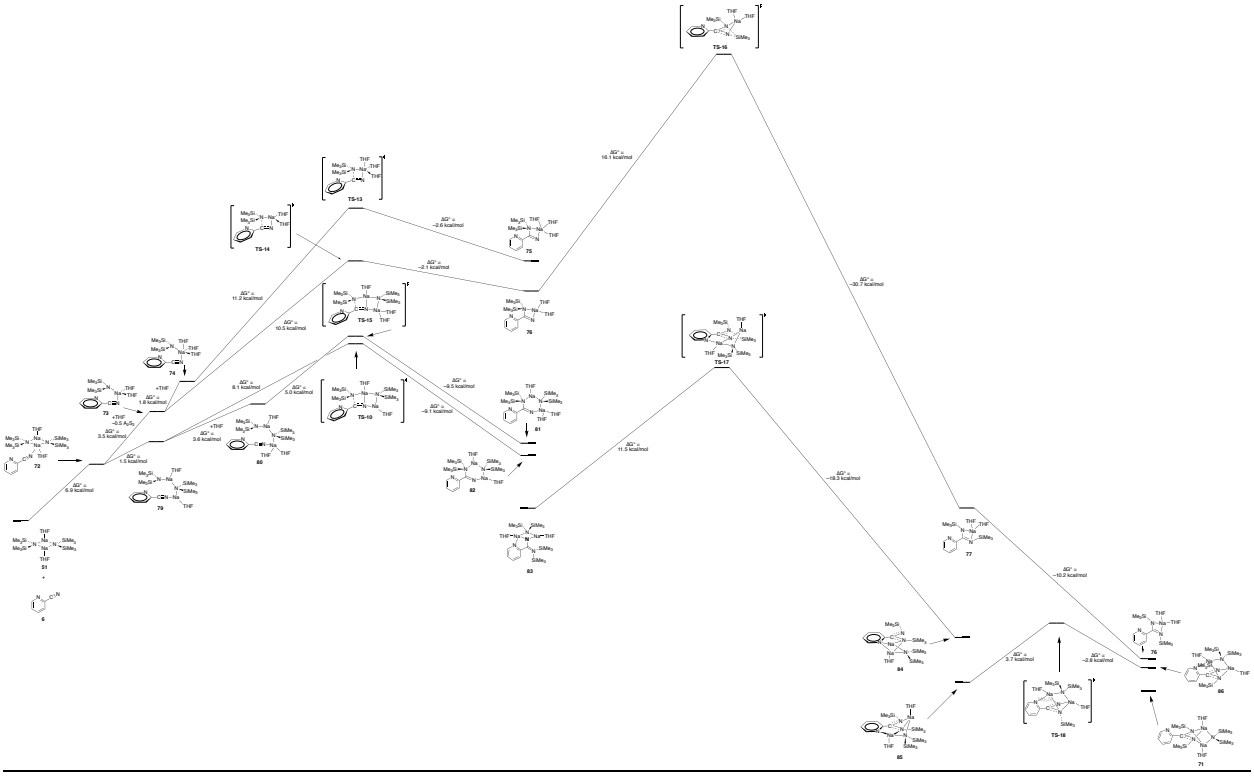
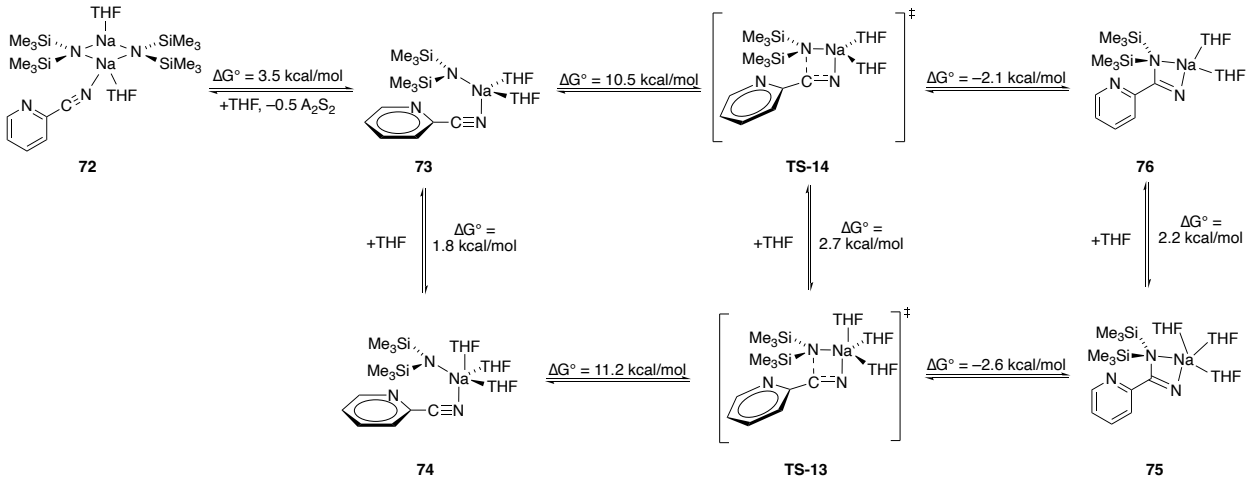
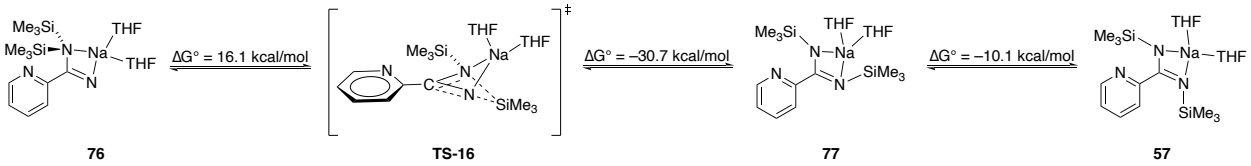


Figure S84. DFT-computed reaction coordinate 1,2-addition of 2-pyridinecarbonitrile (**6**) by NaHMDS in THF.

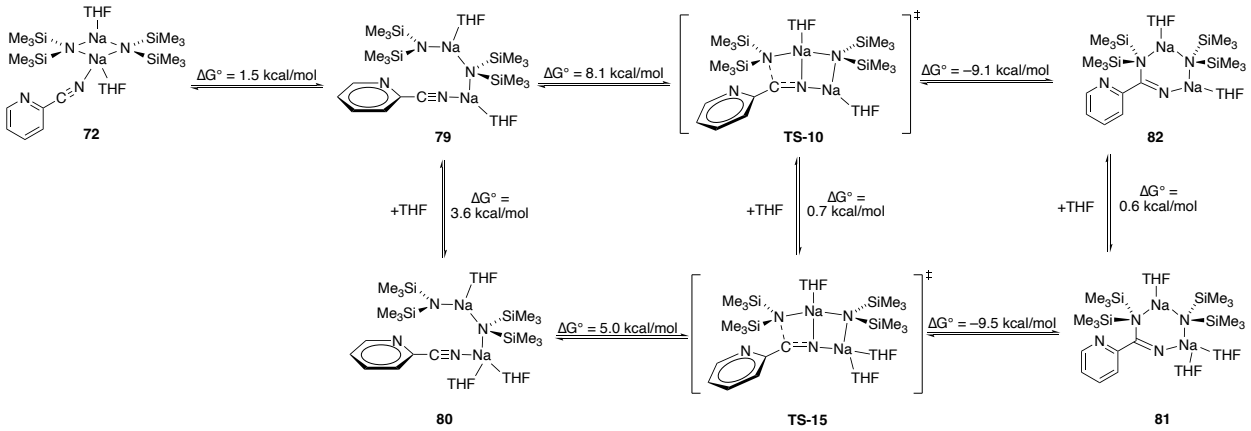
DFT-computed energy profile of 1,2-addition by picolinonitrile (6) and NaHMDS, and subsequent amidine formation in THF via a monomer or dimer pathway



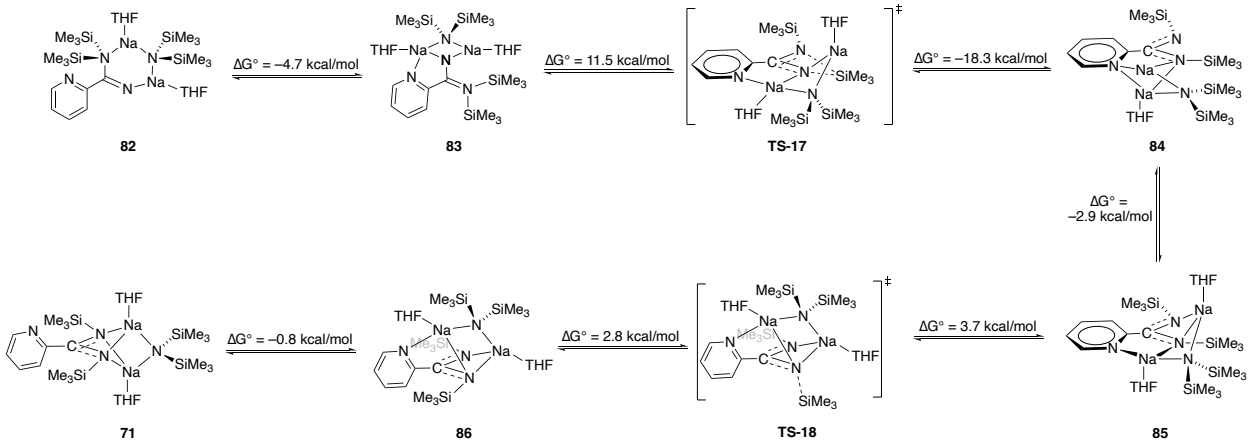
Scheme S4. DFT-computed energy profile of 1,2-addition of picolinonitirile (**6**) by NaHMDS in THF via a monomer pathway.



Scheme S5. DFT-computed energy profile of amidine (**57**) formation via a monomer pathway starting from disolvated monomer pre-silyl-transfer amidinate **76**.



Scheme S6. DFT-computed energy profile of 1,2-addition of picolinonitrile (**6**) by NaHMDS in THF via a dimer pathway.



Scheme S7. DFT-computed energy profile of amidine (**71**) formation via a dimer pathway starting from disolvated monomer pre-silyl-transfer amidinate **82**.

DFT-computed reaction coordinate 1,2-Addition of 2-pyridinecarbonitrile (6) by NaHMDS in DMEA using Me_3N as a DMEA surrogate.

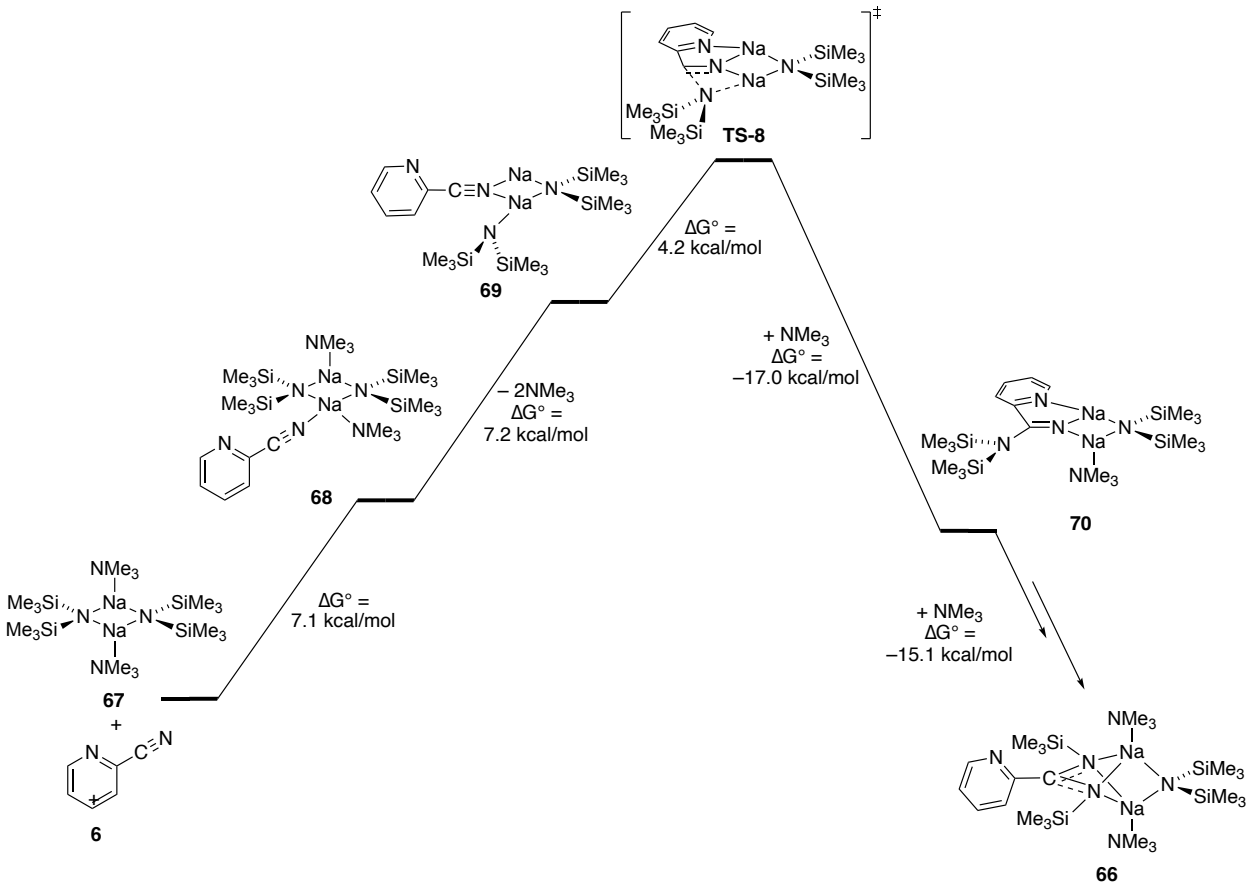
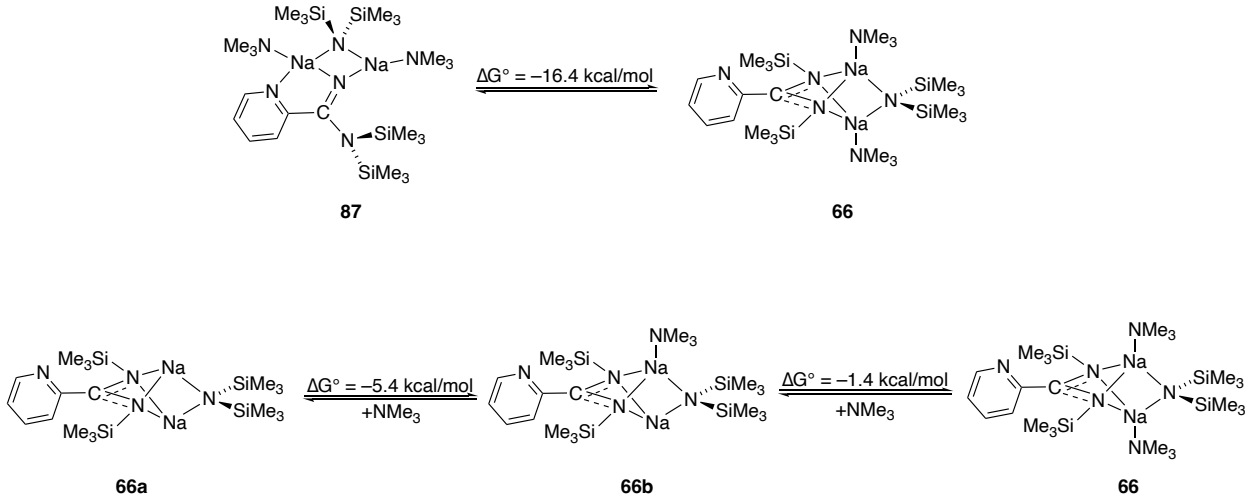


Figure S85. DFT-computed reaction coordinate 1,2-addition of 2-pyridinecarbonitrile (**6**) by NaHMDS in DMEA using Me_3N as a DMEA surrogate.

DFT-computed ground state structures of mixed aggregate

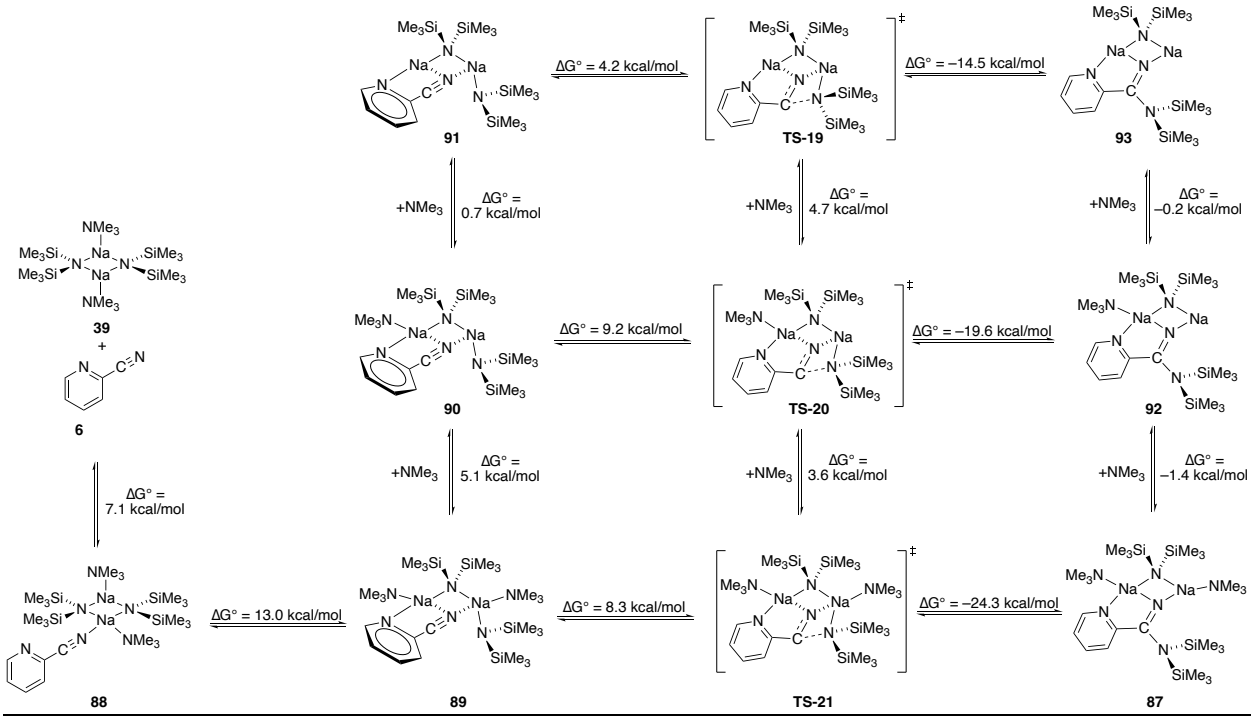


87 66

66a 66b 66

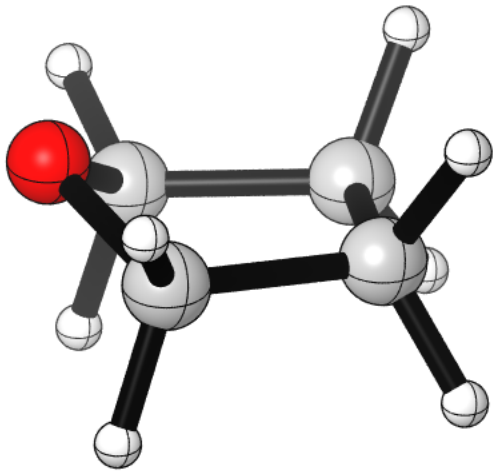
Scheme S8. DFT-computed free energies for the mixed aggregate **66** and serial solvation of mixed aggregate **66** with DMEA using Me_3N as a surrogate.

DFT-computed energy profile of 1,2-addition by picolinonitrile (6) and NaHMDS in DMEA



Scheme S9. DFT-computed energy profile of 1,2-addition of picolinonitrile (**6**) by NaHMDS in DMEA via a dimer pathway using Me_3N as a DMEA surrogate.

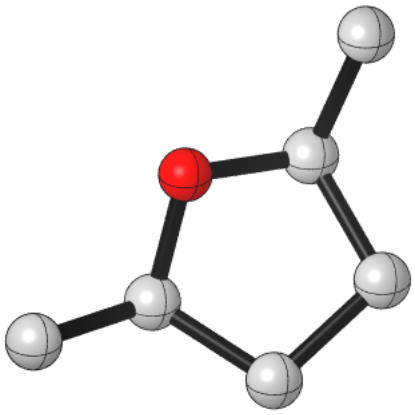
Table S11. Atomic coordinates and single point energies for THF.



G = –232.078328
G_{SP} = –232.348175

C	-1.13117800	-0.46076700	0.13845600
O	-0.01005700	-1.18800400	-0.29984600
C	1.11055700	-0.48578900	0.17603900
C	0.78898700	0.99574800	-0.07428100
C	-0.75601300	1.02638800	-0.02478700
H	-2.00050600	-0.76807500	-0.45672800
H	-1.34061400	-0.68810200	1.20168600
H	1.24953400	-0.67214400	1.25943200
H	2.00145600	-0.84580900	-0.35409600
H	1.25610000	1.65352600	0.67003800
H	1.15027000	1.30071600	-1.06523800
H	-1.14029100	1.63287200	0.80571300
H	-1.16961500	1.43756200	-0.95460100

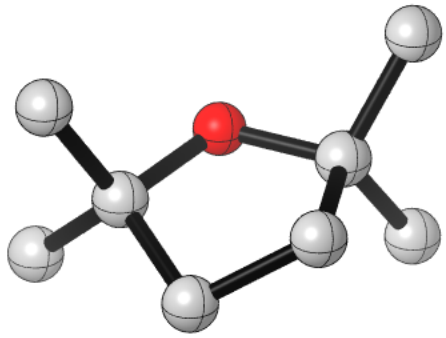
Table S12. Atomic coordinates and single point energies for 2,5-Me_2THF.



G = –310.558747
G_{SP} = –310.914859

C	-1.13141200	-0.11493300	-0.38014700
O	0.00003300	-0.89724700	-0.06597800
C	1.13142900	-0.11481800	-0.38010000
C	0.77083900	1.30399600	0.10522300
C	-0.77095200	1.30401100	0.10497000
H	-1.25515500	-0.09384400	-1.48258100
H	1.25513000	-0.09361800	-1.48252800
H	1.16387100	1.46046200	1.12012200
H	1.20434700	2.07725100	-0.54279600
H	-1.16436400	1.46087400	1.11965800
H	-1.20420300	2.07704100	-0.54348900
C	-2.35884400	-0.72520000	0.25839300
H	-3.25066300	-0.12255400	0.03669100
H	-2.52126000	-1.74497100	-0.11514200
H	-2.22283100	-0.77138700	1.34849200
C	2.35892000	-0.72513300	0.25829500
H	2.52119500	-1.74490900	-0.11530100
H	3.25076000	-0.12255500	0.03649900
H	2.22303400	-0.77135300	1.34840200

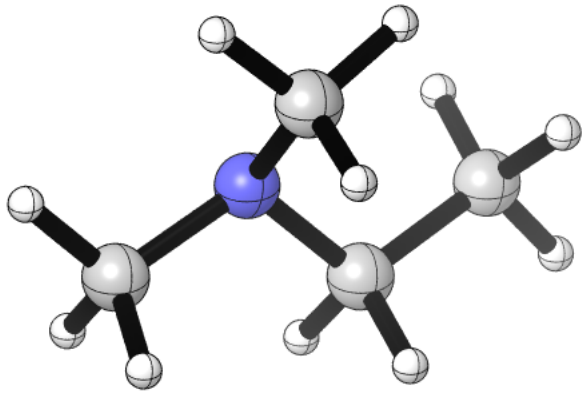
Table S13. Atomic coordinates and single point energies for 2,2,5,5-Me_4THF.



G = –389.044351
G_{SP} = –389.4868685

C	-1.18822700	-0.01098900	-0.08042100
O	-0.00004200	-0.00018800	-0.87272400
C	1.18827500	0.01091700	-0.08046100
C	0.70144700	0.30012400	1.35094300
C	-0.70140700	-0.30028100	1.35095100
H	1.36619000	-0.13181800	2.11172900
H	0.65759400	1.38694700	1.52013200
H	-0.65756200	-1.38711000	1.52011800
H	-1.36611500	0.13166700	2.11176000
C	-2.11057500	-1.09371000	-0.62332000
H	-3.02897400	-1.16298200	-0.02215900
H	-2.38717500	-0.86911000	-1.66315500
H	-1.59853300	-2.06607800	-0.60515100
C	1.84749500	-1.36436600	-0.18178500
H	2.01717200	-1.61172100	-1.23894400
H	2.81187700	-1.38242100	0.34674000
H	1.19750600	-2.14046300	0.24851200
C	-1.84724900	1.36446600	-0.18165800
H	-2.01697500	1.61182800	-1.23880700
H	-2.81152500	1.38268700	0.34703000
H	-1.19704300	2.14044000	0.24854500
C	2.11028300	1.09393100	-0.62330000
H	3.02858300	1.16352100	-0.02199900
H	2.38719500	0.86946400	-1.66307800
H	1.59787800	2.06610100	-0.60516500

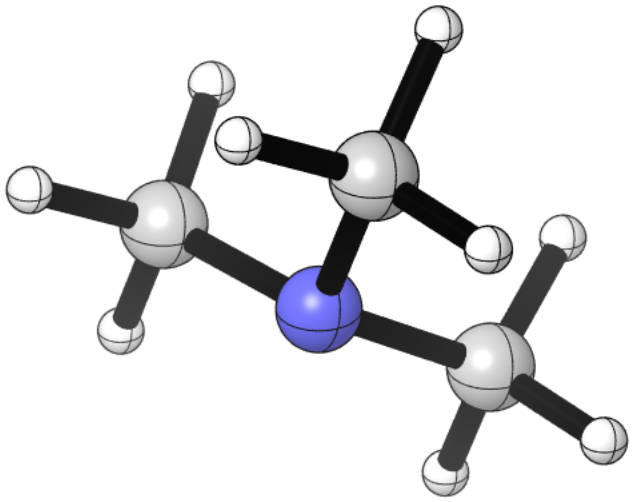
Table S14. Atomic coordinates and single point energies for DMEA.



G = –213.385949
G_{SP} = –213.632267

N	-0.45720800	-0.00327800	-0.31588300
C	-1.66546400	-0.75**25**9200	-0.06018300
C	0.69850700	-0.65063500	0.27782000
C	2.02409400	-0.03226900	-0.14249600
C	-0.60214100	1.37503500	0.09391400
H	-2.51572500	-0.28597700	-0.57818000
H	-1.91612100	-0.81051900	1.02298700
H	-1.55962600	-1.77996100	-0.43743900
H	0.68127900	-1.70499400	-0.03975600
H	0.62391500	-0.65864400	1.39094800
H	2.06820700	0.04904100	-1.23791100
H	2.86040800	-0.65862100	0.19692600
H	2.17020900	0.96941000	0.28492100
H	-1.48654000	1.81399300	-0.38940500
H	0.26992500	1.96809000	-0.21178100
H	-0.72545000	1.48389400	1.19554700

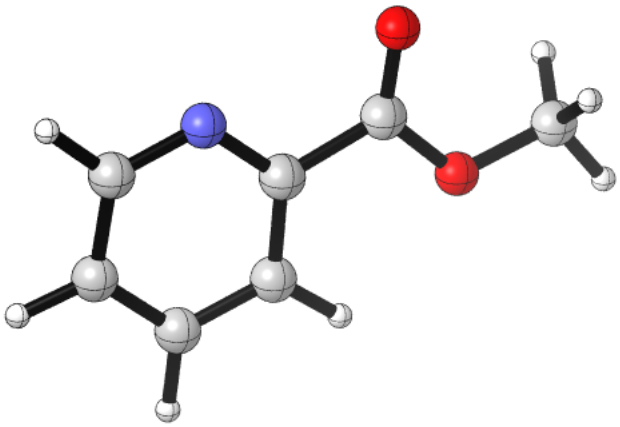
Table S15. Atomic coordinates and single point energies for Me_3N.



G = –174.146930
G_{SP} = –174.349420

N	0.00000000	0.00000000	0.36503400
C	0.00000000	1.38014100	-0.05831500
H	-0.88959600	1.89515600	0.33235600
H	0.88959600	1.89515600	0.33235600
H	0.00000000	1.49077800	-1.16656600
C	1.19523800	-0.69007100	-0.05831500
H	2.08605200	-0.17716500	0.33235600
H	1.19645600	-1.71799100	0.33235600
H	1.29105200	-0.74538900	-1.16656600
C	-1.19523800	-0.69007100	-0.05831500
H	-1.19645600	-1.71799100	0.33235600
H	-2.08605200	-0.17716500	0.33235600
H	-1.29105200	-0.74538900	-1.16656600

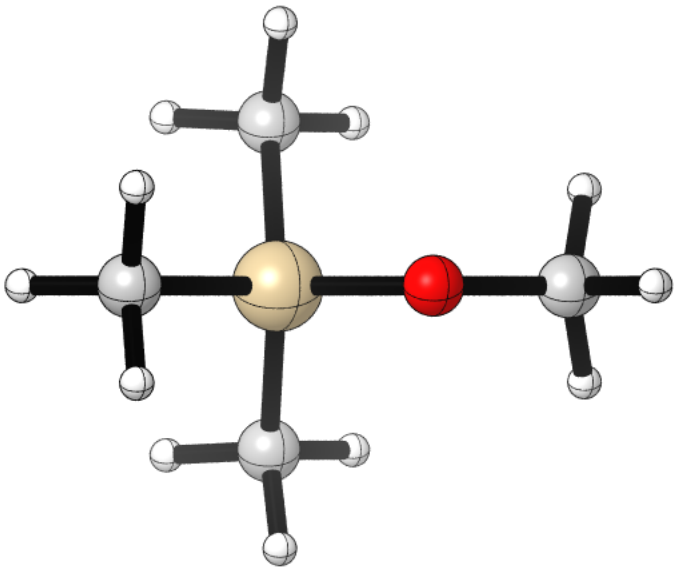
Table S16. Atomic coordinates and single point energies for **3**.



G = –475.508936
G_{SP} = –476.048857

N	1.04291200	1.21578000	-0.00025800
C	2.35664500	1.03245700	-0.00026000
C	0.26139800	0.13834000	0.00003000
C	2.95563200	-0.23074100	-0.00000400
C	0.75301000	-1.17036800	0.00017000
C	2.13370900	-1.35300900	0.00018500
H	2.97497600	1.93514500	-0.00049500
H	4.04204400	-0.32324700	0.00007800
H	2.55948700	-2.35756500	0.00039100
H	0.06052000	-2.01018000	0.00021600
C	-1.22181700	0.41340100	0.00014200
O	-1.71973100	1.50034100	0.00049600
O	-1.93269500	-0.72487600	-0.00028800
C	-3.34168700	-0.56051200	-0.00021900
H	-3.66395700	-0.00500700	0.89080400
H	-3.77102100	-1.56700400	-0.00079000
H	-3.66437100	-0.00372900	-0.89032700

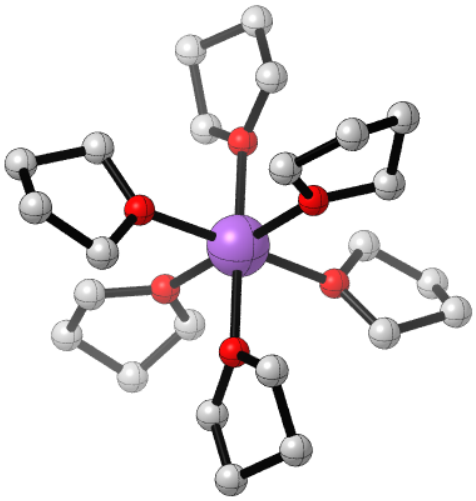
Table S17. Atomic coordinates and single point energies for **TMSOMe**.



G = –523.905424
G_{SP} = –524.287985

Si	-0.38203600	-0.00008400	-0.00686000
C	-0.46829600	1.53438700	-1.08719900
C	-1.73483400	0.00367700	1.27950600
C	-0.46881600	-1.54012500	-1.07912000
H	-1.65619500	0.89482600	1.91894100
H	-1.65676500	-0.88408100	1.92371400
H	-2.73001200	0.00274000	0.81062800
H	-0.35880200	2.44501100	-0.47954200
H	-1.43583000	1.58833800	-1.60924600
H	0.32164900	1.53837100	-1.85342200
H	-0.36307500	-2.44784800	-0.46648100
H	0.32304000	-1.54997100	-1.84329600
H	-1.43517600	-1.59452900	-1.60332200
O	1.05456700	0.00211100	0.85532000
C	2.31637000	0.00055700	0.25060300
H	2.47416600	-0.89457000	-0.37761500
H	3.08842000	0.00278900	1.03292800
H	2.47399600	0.89223400	-0.38254800

Table S18. Atomic coordinates and single point energies for $^{+}$**Na(THF)$_6$**.



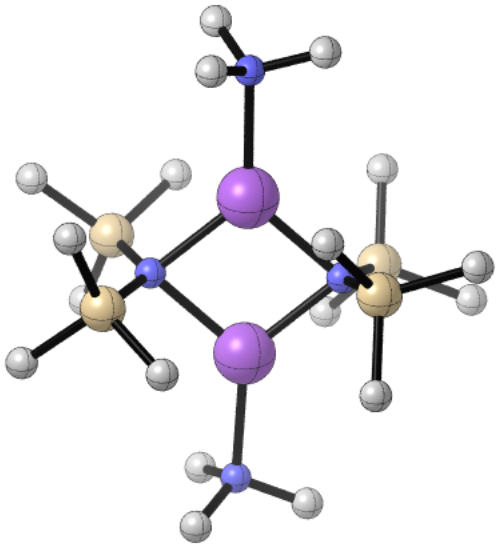
G = –1554.573195
G_{SP} = –1556.202536

Na	-0.01521300	-0.00921800	-0.00300000
O	1.73780200	0.63700600	1.29003100
O	1.43561400	-1.05223900	-1.39587100
O	0.17673800	1.87362300	-1.26688300
O	-1.76768100	-0.64501600	-1.29761100
O	-1.46913100	0.98253800	1.42031400
O	-0.19534100	-1.89084700	1.25887100
C	-0.67003300	2.21755900	-2.36165900
C	0.98722000	2.98613200	-0.88942500
C	-0.70786100	3.73992800	-2.36997800
C	0.71805300	4.07273000	-1.92984400
H	-1.64560800	1.73546100	-2.20539100
H	-0.23761900	1.82721500	-3.30050000
H	-1.43477400	4.10866800	-1.62984100
H	-0.97413500	4.15614600	-3.34939600
H	0.83023000	5.08541600	-1.52348600
H	1.40879400	3.96825700	-2.77960400
H	0.69560900	3.30947600	0.12478300
H	2.04170800	2.67214900	-0.85888200
C	1.92540600	-0.48661400	-2.61192800
C	2.28517100	-2.10482600	-0.94637100
C	3.56931400	-1.96250100	-1.75565200
C	3.03119800	-1.42656400	-3.08328200
H	1.09096200	-0.39906300	-3.32336500
H	2.30607800	0.52962100	-2.40806800
H	3.78878700	-0.91902300	-3.69298500

H	2.60693400	-2.24803700	-3.67953100
H	4.23735900	-1.22392700	-1.28649400
H	4.11884400	-2.90700700	-1.85231900
H	2.42577100	-1.99846900	0.13983900
H	1.79892100	-3.07773600	-1.14067400
C	1.52663000	1.32701500	2.52468600
C	3.10698500	0.70378400	0.90633900
C	2.91354400	1.75079500	3.00646300
C	3.68184400	1.87587000	1.68993400
H	3.15402700	0.81730100	-0.18720800
H	3.61888000	-0.23821400	1.17781700
H	3.43648500	2.82567700	1.19040100
H	4.77094800	1.81977300	1.80842400
H	2.89216500	2.67681100	3.59397000
H	3.36101500	0.96274100	3.63009700
H	1.01131300	0.65414500	3.22684400
H	0.86934900	2.19200400	2.33677100
C	0.63252000	-2.27855000	2.35187400
C	-0.89807500	-3.01753700	0.73466400
C	0.79957100	-3.78544000	2.20752900
C	-0.57507500	-4.18379800	1.66838800
H	1.56930500	-1.70528600	2.29035400
H	0.13165800	-2.02827800	3.30470100
H	-1.97290200	-2.78452600	0.68976600
H	-0.54489600	-3.20526800	-0.29424000
H	1.06170000	-4.27969300	3.15115200
H	1.58351200	-4.01341100	1.46918400
H	-0.58330800	-5.15275200	1.15416400
H	-1.30384400	-4.22903200	2.49099400
C	-2.09722300	2.23365200	1.15846000
C	-2.06005100	0.34697300	2.55493000
C	-3.41734900	2.18384100	1.91665600
C	-3.01708600	1.37609600	3.15189200
H	-1.26437800	0.03684900	3.24766900
H	-2.58904000	-0.56153000	2.22063200
H	-2.48816700	2.02096400	3.86942100
H	-3.86594200	0.91437500	3.67104800
H	-3.81552100	3.17906900	2.14984000
H	-4.17310100	1.63840100	1.33057300
H	-2.20464700	2.34747200	0.06935600
H	-1.45807400	3.05534100	1.53013600
C	-3.14139000	-0.50472900	-0.93660400
C	-1.63839200	-1.44688300	-2.46924700
C	-3.93917500	-1.25392200	-2.00703100

C	-2.91719000	-2.26996800	-2.52010100
H	-3.39942500	0.56516800	-0.88355400
H	-3.28619500	-0.93828100	0.06710500
H	-4.22798300	-0.56985500	-2.81839400
H	-4.85364900	-1.71054800	-1.60898100
H	-3.14399000	-2.65002600	-3.52389100
H	-2.84391400	-3.12776700	-1.83414100
H	-1.55388200	-0.79489000	-3.35830100
H	-0.71335500	-2.03326300	-2.37774800

Table S19. Atomic coordinates and single point energies for **39**.



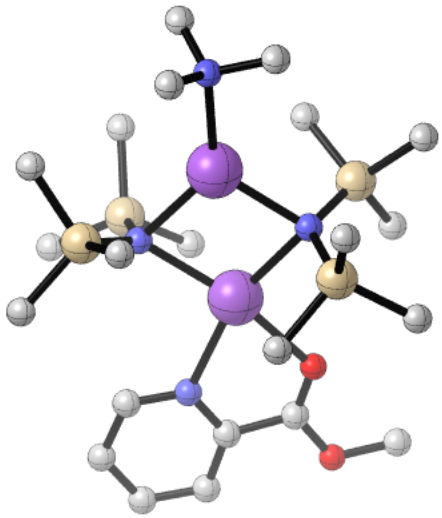
G = –2417.956178
G_{SP} = –2419.545983

Na	-1.26548900	-0.77739100	-0.01634900
Na	1.33486000	0.67616800	0.00877400
N	-0.84573600	1.52384000	-0.00253900
N	0.91718400	-1.61484600	-0.00711300
Si	-0.83863900	2.46738700	-1.43034500
C	0.63414700	1.96176400	-2.52729700
C	-0.62009100	4.32955700	-1.13174800
C	-2.38827400	2.24408300	-2.49917300
Si	-1.63439700	2.00811600	1.43686000
C	-1.93684600	0.49014200	2.54582200
C	-3.34657700	2.78065100	1.15945300
C	-0.62680400	3.22290900	2.48698900
Si	1.25216600	-2.22042200	-1.56346100
C	2.77179100	-1.38155100	-2.34007900
C	-0.23072100	-1.87698900	-2.71567100
C	1.56127600	-4.08466100	-1.68752000
Si	1.22889600	-2.26684600	1.53529800
C	1.73530300	-0.87467500	2.73923700
C	2.62218300	-3.54561300	1.63715800
C	-0.31364500	-3.10815500	2.26451900
H	-2.47424600	1.20060200	-2.84350500
H	-2.36774100	2.88963000	-3.39108300
H	-3.29548500	2.48713400	-1.92371000
H	1.59947400	2.19692300	-2.04940600

H	0.61561100	2.51082600	-3.48145400
H	0.62706700	0.88771200	-2.77165300
H	0.32350700	4.52428700	-0.59611100
H	-1.43630400	4.74551600	-0.52059600
H	-0.59294000	4.88902400	-2.07992100
H	-4.00159400	2.08092000	0.61480000
H	-3.28586600	3.70360300	0.56176700
H	-3.83676500	3.03113700	2.11326400
H	0.31877700	2.75783200	2.81053500
H	-1.17247200	3.53459200	3.39129400
H	-0.37937100	4.12737700	1.90950700
H	-2.63352900	-0.22741500	2.08290000
H	-2.38970900	0.79166800	3.50305700
H	-1.00466400	-0.04648900	2.78293200
H	0.75740900	-4.65086600	-1.18959000
H	2.51382700	-4.36642800	-1.21439500
H	1.60044500	-4.40543300	-2.74052600
H	-0.62351700	-0.85012800	-2.61715100
H	-1.04985200	-2.57995000	-2.49060400
H	0.03073900	-2.02019500	-3.77567800
H	2.69058100	-0.28085800	-2.33882700
H	2.93449800	-1.69690000	-3.38256600
H	3.66869400	-1.65530000	-1.76071800
H	-1.18773900	-2.43444300	2.28653000
H	-0.15011500	-3.46549700	3.29322800
H	-0.57352800	-3.97956500	1.64125900
H	3.53457900	-3.17191700	1.14459200
H	2.33887000	-4.48987400	1.14867700
H	2.87073000	-3.77067300	2.68636700
H	2.79081200	-0.60030100	2.57813700
H	1.64454600	-1.19221100	3.78985700
H	1.12373300	0.03714800	2.62616000
N	-3.44270400	-1.85905400	-0.18735000
N	3.44329800	1.87068600	0.21917900
C	-3.87068300	-1.27181500	-1.45132900
C	-4.43863300	-1.61110200	0.84505700
C	-3.20446400	-3.28973600	-0.32614000
H	-4.83484800	-1.69694900	-1.79752300
H	-3.11625500	-1.45624200	-2.23003100
H	-3.98939900	-0.18438000	-1.33651300
H	-5.41037200	-2.08255500	0.59254100
H	-4.59807200	-0.53023000	0.96320200
H	-4.09465500	-2.01866600	1.80606300
H	-4.11748300	-3.82768100	-0.65375200

H	-2.87889100	-3.70666300	0.63649400
H	-2.41068200	-3.47493700	-1.06396100
C	3.23589600	2.51911100	1.50794100
C	3.80079500	2.85580700	-0.79061500
C	4.46901100	0.83969600	0.30911600
H	4.75209100	3.36829200	-0.53997700
H	3.01006400	3.61469100	-0.87304300
H	3.91714000	2.36758100	-1.76841600
H	2.42365200	3.25636900	1.42901600
H	4.15042900	3.03954000	1.85879100
H	2.95437600	1.77385000	2.26609900
H	4.16458100	0.06100800	1.02316900
H	5.44227000	1.25670300	0.63956300
H	4.60585800	0.36603200	-0.67225600

Table S20. Atomic coordinates and single point energies for **40**.



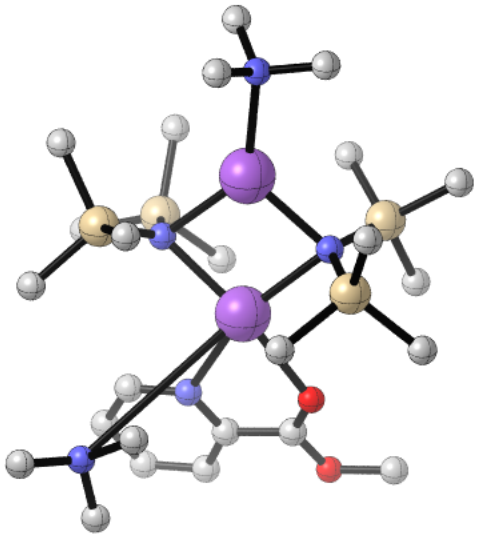
G = –2719.329639
G_{SP} = –2721.253393

N	-0.41817600	-1.83088300	-0.11746100
N	-0.82145000	1.79253900	0.10244300
Na	0.88303200	0.15069400	0.02203900
Na	-2.05787800	-0.13299000	-0.11278100
Si	-0.14015000	-2.32844400	-1.72915800
C	-1.73961800	-2.42958300	-2.75587300
C	0.69434400	-4.02310900	-1.92375200
C	0.99747600	-1.07610700	-2.60494400
Si	-1.01089200	-2.85134700	1.11529000
C	-2.51996400	-3.87194300	0.55869200
C	-1.56313900	-1.83346500	2.62848600
C	0.22490200	-4.11730600	1.81018100
Si	-0.41813400	2.47655800	1.61378000
C	0.70302100	1.27804400	2.58702900
C	-1.93875800	2.79762000	2.70309700
C	0.57579800	4.09035100	1.51490700
Si	-1.16932300	2.68350800	-1.30946000
C	-2.31658000	4.17530000	-1.04850900
C	-2.05969000	1.54851600	-2.56044500
C	0.36903200	3.33616900	-2.20696500
H	0.61922200	-0.04098600	-2.54437600
H	1.09397400	-1.31509900	-3.67512400
H	2.01091300	-1.09435700	-2.17141600
H	0.07093400	-4.82210000	-1.49128300
H	1.67423000	-4.05282400	-1.42120900

H	0.85506300	-4.26389900	-2.98639600
H	-2.39491300	-3.22145900	-2.35967500
H	-1.53485600	-2.65906400	-3.81362000
H	-2.30670900	-1.48389800	-2.73068500
H	-0.27721600	-4.80494000	2.50903600
H	1.03509300	-3.61840100	2.36524700
H	0.67518900	-4.72374800	1.00829100
H	-3.28995000	-3.22465200	0.10688100
H	-2.98197800	-4.42166200	1.39408600
H	-2.23126800	-4.60885500	-0.20850300
H	-2.27514600	-2.39957700	3.24971800
H	-2.04140700	-0.87262800	2.37241500
H	-0.69564800	-1.59344200	3.26247800
H	1.50161000	3.89787000	0.94968400
H	0.84878000	4.45787000	2.51674500
H	0.02476000	4.89208300	0.99971300
H	-2.48305900	1.85606000	2.88781500
H	-2.62755400	3.49363300	2.19752300
H	-1.67462300	3.22973800	3.68089500
H	0.30074700	0.25184400	2.59465100
H	0.80409300	1.59499800	3.63626800
H	1.72020900	1.25158300	2.16021800
H	0.91843200	4.03096500	-1.55242500
H	0.10931800	3.86803400	-3.13584500
H	1.05479700	2.51155200	-2.45837600
H	-3.02474800	1.17293900	-2.17709800
H	-1.44056300	0.67684100	-2.82800500
H	-2.28171500	2.08515000	-3.49574200
H	-3.25893300	3.87242800	-0.56593100
H	-2.56402500	4.66681200	-2.00269000
H	-1.84404200	4.92848300	-0.39884900
N	3.00720800	-0.94863400	0.30968900
C	3.14237600	-2.24935100	0.53800300
C	4.10058200	-0.19843900	0.17601800
C	4.39657800	-2.85784700	0.65471800
C	5.39412300	-0.70602800	0.27620100
C	5.53692300	-2.07161800	0.52405400
H	2.21150800	-2.81739100	0.62404200
H	4.46494700	-3.92926500	0.84323100
H	6.53004400	-2.51474500	0.60992600
H	6.25070200	-0.04398200	0.15865200
O	2.69902600	1.68515600	-0.24354200
C	3.81624200	1.24989000	-0.11314600
O	4.90987000	1.98750400	-0.21448700

C	4.70350100	3.37092200	-0.49654700
H	5.69893200	3.81336600	-0.59002900
H	4.14466700	3.84309500	0.32186000
H	4.13412100	3.48662400	-1.42772200
N	-4.45243100	-0.10413200	0.20875600
C	-5.12942500	-0.76050200	-0.90097600
H	-4.83134500	-0.29918100	-1.85354000
H	-4.85570500	-1.82473900	-0.93368400
H	-6.23251200	-0.68638700	-0.80937500
C	-4.81152900	-0.73585600	1.47158600
H	-4.49162800	-1.78783300	1.47648600
H	-4.31354800	-0.21954300	2.30411000
H	-5.90637500	-0.69805700	1.64672700
C	-4.77003700	1.31857300	0.24609800
H	-4.17916300	1.81533000	1.02930800
H	-4.51810600	1.78668300	-0.71551400
H	-5.84744300	1.49123500	0.44571400

Table S21. Atomic coordinates and single point energies for **44b**.



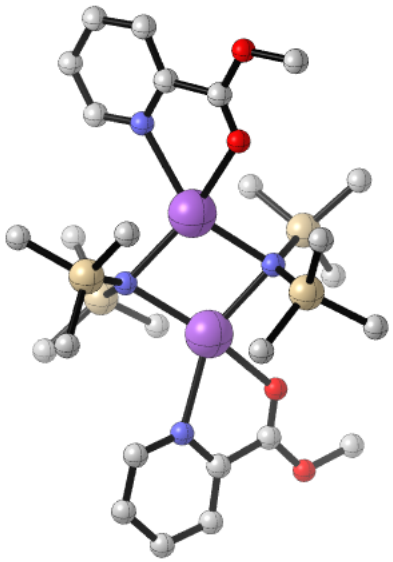
G = –2893.468015
G_{SP} = –2895.592055

N	0.17973200	1.71913500	-0.50238400
N	1.78504100	-1.45521600	0.38613800
Na	2.28428400	0.73073300	-0.13827600
Na	-0.38540500	-0.48266300	0.15093300
Si	0.02966000	1.84444100	-2.20172200
Si	0.11057900	3.05599500	0.55748400
C	-0.50081900	0.18000900	-2.96816000
C	1.67718900	2.34460200	-3.01982800
C	-1.21894600	3.12788500	-2.83891500
C	-1.62484300	3.78009000	0.81596500
C	1.20606800	4.51009100	-0.00174900
C	0.72767800	2.57374000	2.29310200
Si	1.60763000	-2.08768700	1.96504800
Si	2.49989900	-2.34480600	-0.88341000
C	3.12877700	-1.77871500	3.05787400
C	1.20887000	-3.94200600	2.04224100
C	0.13826900	-1.24669900	2.83667100
C	1.33470000	-3.61918300	-1.67531700
C	4.07570300	-3.29419600	-0.40505600
C	3.02302100	-1.16657700	-2.28842000
H	-2.24169000	2.92015700	-2.48824500
H	-1.23721300	3.12835200	-3.94046100
H	-0.95092300	4.14440800	-2.50984800
H	2.50388700	1.66029900	-2.76743900

H	1.96387200	3.35357200	-2.68180800
H	1.60055400	2.36597400	-4.11859100
H	-0.07664900	-0.69005300	-2.43746400
H	-0.16957300	0.10692400	-4.01609700
H	-1.59729800	0.07619800	-2.96139600
H	-2.02997300	4.17563400	-0.12942500
H	-1.60706000	4.60713700	1.54406400
H	-2.32535800	3.01374800	1.18650200
H	0.85055100	4.92914500	-0.95682700
H	2.24666600	4.18128700	-0.16187000
H	1.21785700	5.32603900	0.73805500
H	-0.04715700	2.02575300	2.85153200
H	0.98010600	3.46932300	2.88252200
H	1.62325900	1.92963700	2.27365600
H	4.83726800	-2.61329700	0.00616400
H	4.51377500	-3.80734900	-1.27579100
H	3.86988600	-4.05656300	0.36230400
H	1.03469100	-4.35815800	-0.91565300
H	1.81223600	-4.15398400	-2.51131600
H	0.42102800	-3.13177500	-2.05199200
H	2.16281700	-0.62561600	-2.71310900
H	3.49065100	-1.72802200	-3.11206000
H	3.76603900	-0.41935600	-1.95684600
H	0.18781900	-0.14825900	2.75947900
H	0.11727600	-1.49504100	3.90888500
H	-0.81602600	-1.59642400	2.40822800
H	2.00104600	-4.56465300	1.59889100
H	0.27672100	-4.12576200	1.48471800
H	1.06215000	-4.27436700	3.08210800
H	4.02351900	-2.24152500	2.61137700
H	3.00522000	-2.18664500	4.07324800
H	3.31775700	-0.69613100	3.15170600
N	4.50769500	1.56097600	0.25796300
C	5.32237200	0.37072000	0.46812700
C	4.44844000	2.35720800	1.47606400
C	5.01429400	2.35395500	-0.85249400
H	5.44872300	2.74324800	1.76099500
H	4.07117200	1.74296000	2.30623000
H	3.77043200	3.21236500	1.34061800
H	6.04534200	2.71617000	-0.66120300
H	4.36551300	3.22537900	-1.02102400
H	5.02509200	1.75158700	-1.77230800
H	4.86980300	-0.26159900	1.24591000
H	6.35594100	0.63195700	0.77484700

H	5.37596700	-0.21701700	-0.45880200
N	-2.71062400	-0.27486800	-0.51692200
C	-3.30745200	0.87636600	-0.79930700
C	-3.28574100	-1.41350000	-0.90669900
C	-4.52178100	0.93261400	-1.49358600
C	-4.48999000	-1.46643100	-1.60393600
C	-5.11857700	-0.25527100	-1.89995300
H	-2.79120800	1.78086600	-0.47224000
H	-4.97797800	1.89918200	-1.70803500
H	-6.06272500	-0.24455100	-2.44646000
H	-4.90669100	-2.42704400	-1.90265900
C	-2.50538200	-2.64591100	-0.54356300
C	-2.34935600	-4.96737400	-0.68185800
O	-1.46717100	-2.60595600	0.07088500
O	-3.06428400	-3.76593100	-0.96964300
H	-2.27238600	-5.10961300	0.40407100
H	-1.33889300	-4.91381100	-1.10737500
H	-2.92371400	-5.77840700	-1.13768200
N	-4.13740400	1.30400000	2.12323900
C	-5.27596000	0.45552800	1.85804500
C	-4.49806500	2.44507400	2.93554500
C	-3.03814100	0.56072800	2.69705100
H	-4.98152200	-0.37418800	1.19629600
H	-6.06690700	1.03012700	1.35282000
H	-5.70840300	0.01717500	2.78461800
H	-3.62504400	3.09885200	3.07319100
H	-4.87149300	2.14914200	3.94054700
H	-5.28530900	3.02909500	2.43702900
H	-2.14836900	1.20414400	2.77578500
H	-2.78526000	-0.28966000	2.04732900
H	-3.26764400	0.16346300	3.71024000

Table S22. Atomic coordinates and single point energies for **41**.



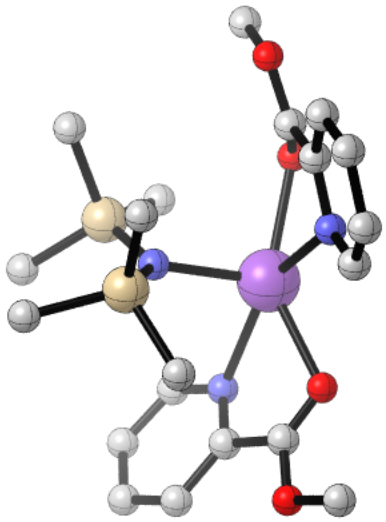
G = –3020.706276
G_{SP} = –3022.964298

N	-0.00114400	1.78388100	0.00070500
N	0.00021400	-1.83840200	0.00122600
Na	1.50615300	0.00919000	-0.00372900
Na	-1.50705500	0.00826500	0.00798600
Si	-0.47843500	2.55769300	-1.43498400
C	0.96634000	3.10032800	-2.54011300
C	-1.58611100	4.08048300	-1.17204500
C	-1.53867100	1.35622100	-2.47856800
Si	0.47790300	2.56017100	1.43452300
C	1.53707500	1.35965500	2.48032900
C	-0.96562800	3.10681700	2.53915600
C	1.58772100	4.08064800	1.16744400
Si	-0.56682500	-2.61552900	1.40804400
C	-1.64959400	-4.14715900	1.09383100
C	-1.65709300	-1.42322200	2.42121700
C	0.80232100	-3.19551500	2.59198800
Si	0.56822500	-2.61396200	-1.40604300
C	1.65740600	-1.41970500	-2.41815400
C	-0.79987600	-3.19480000	-2.59080300
C	1.65243100	-4.14483300	-1.09295200
H	-1.06182000	4.86936100	-0.60963800
H	-2.46818400	3.78064000	-0.58376600
H	-1.93083400	4.51518300	-2.12362900
H	1.60772300	3.80729100	-1.98979800

H	0.62247500	3.58892400	-3.46550900
H	1.59012200	2.23336400	-2.80890600
H	-1.04741300	0.37633400	-2.61166000
H	-1.72901900	1.76222200	-3.48389300
H	-2.52416500	1.18395400	-2.01150600
H	-1.59016600	2.24101400	2.80989800
H	-1.60652600	3.81346100	1.98788000
H	-0.62074900	3.59681300	3.46343400
H	2.46841700	3.77758100	0.57877100
H	1.93431100	4.51658700	2.11777900
H	1.06427600	4.86934900	0.60400600
H	1.04479300	0.38057800	2.61556900
H	1.72784800	1.76757700	3.48479600
H	2.52239400	1.18543200	2.01363600
H	1.44405600	-3.94439600	2.09916400
H	0.38278800	-3.65999500	3.49819800
H	1.43186100	-2.34830200	2.90897700
H	-2.62695200	-1.24406400	1.92678500
H	-1.17079700	-0.44654900	2.58745000
H	-1.87825400	-1.84763200	3.41244100
H	-2.55107200	-3.87861500	0.52055000
H	-1.97899500	-4.60652000	2.03932200
H	-1.10521200	-4.91450200	0.52051300
H	2.55372900	-3.87606200	-0.51950300
H	1.98212300	-4.60318900	-2.03883100
H	1.10868700	-4.91306600	-0.52021400
H	-1.43011500	-2.34822800	-2.90807900
H	-1.44114300	-3.94444500	-2.09852900
H	-0.37928800	-3.65872700	-3.49681000
H	1.17027600	-0.44323100	-2.58309400
H	1.87868800	-1.84279200	-3.40991400
H	2.62723700	-1.24042000	-1.92371300
N	-3.76040300	-0.93589500	-0.53396200
C	-4.01651400	-2.08178300	-1.15495800
C	-4.78921400	-0.19434700	-0.11844500
C	-5.31819200	-2.53801800	-1.38621000
C	-6.12217800	-0.55696800	-0.30125000
C	-6.38663800	-1.76170200	-0.95159900
H	-3.14913000	-2.65883600	-1.48374000
H	-5.47697300	-3.48642300	-1.89916000
H	-7.41488800	-2.08691800	-1.11555500
H	-6.91597600	0.09436700	0.06096800
C	-4.39606600	1.08011100	0.57625700
O	-3.24979400	1.39444700	0.76984600

O	-5.43323200	1.81280100	0.95124000
C	-5.11767400	3.03683900	1.61392200
H	-6.07464000	3.48525200	1.89441700
H	-4.56182900	3.69877500	0.93707500
H	-4.50017200	2.84090000	2.49980500
H	4.56208000	3.70173800	-0.93322800
C	4.78874900	-0.19305000	0.11727800
C	5.32045900	-2.53864400	1.38031400
C	6.38794600	-1.76265000	0.94278400
C	6.12208300	-0.55692900	0.29483900
C	4.39413700	1.08266400	-0.57425700
C	5.11331300	3.03941100	-1.61346800
C	4.01831200	-2.08113300	1.15427000
N	3.76084000	-0.93432400	0.53553300
O	3.24738900	1.39867900	-0.76228400
O	5.43047300	1.81442600	-0.95325300
H	5.48033300	-3.48780900	1.89151600
H	6.91508100	0.09423100	-0.06943800
H	7.41652400	-2.08888400	1.10261300
H	6.06948200	3.48655700	-1.89866900
H	3.15169800	-2.65806100	1.48529600
H	4.49080900	2.84499800	-2.49619000

Table S23. Atomic coordinates and single point energies for **42**.

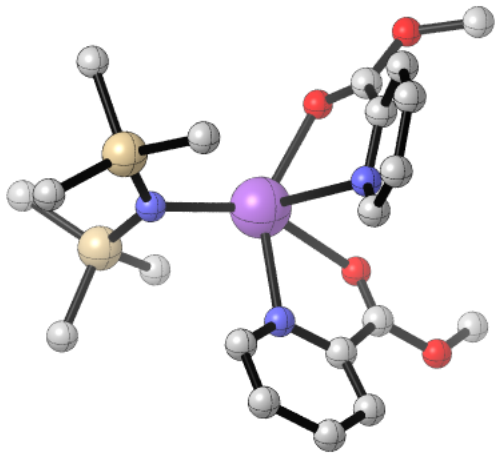


G = –1985.854875
G_{SP} = –1987.520377

N	-0.02441400	-0.92801400	-0.60080000
Si	-0.04312700	-0.10999900	-2.08065600
Si	0.12499900	-2.59751700	-0.37716200
C	-0.98080200	1.54831400	-1.96533300
C	-0.87476400	-1.04690400	-3.51343700
C	1.68225400	0.37865700	-2.72398800
C	1.71518900	-3.32438600	-1.14029600
C	-1.29931000	-3.64603100	-1.08535600
C	0.19717300	-3.06097800	1.47972400
Na	-0.02671100	0.15605500	1.39346400
H	-1.90158800	-1.34084100	-3.24322300
H	-0.32017400	-1.96657200	-3.76190700
H	-0.92147800	-0.42872300	-4.42433000
H	2.13076100	1.15085000	-2.07864500
H	1.64066300	0.78285800	-3.74843100
H	2.35883700	-0.49103600	-2.72462500
H	-2.04883600	1.38874900	-1.74376000
H	-0.91205500	2.11150100	-2.90990000
H	-0.54606700	2.16873000	-1.16551200
H	1.64429400	-3.32091800	-2.24047500
H	1.91980200	-4.35919300	-0.82014200
H	2.58079100	-2.69428900	-0.87596400
H	1.20718400	-2.93616700	1.89422000
H	-0.10539500	-4.10983100	1.62967500
H	-0.46647000	-2.43582000	2.10025900

H	-1.34311000	-3.56055000	-2.18165100
H	-2.26995500	-3.30318300	-0.69219600
H	-1.18127100	-4.71212500	-0.83191800
N	1.76502100	1.75423000	0.81131700
C	1.65250800	2.96167200	0.27302200
C	2.90680200	1.08827600	0.64435600
C	2.68597900	3.56412700	-0.45064900
C	3.99653800	1.59421900	-0.06231700
C	3.87760400	2.86636700	-0.61846500
H	0.69479900	3.46559700	0.43072500
H	2.54868000	4.55885200	-0.87456700
H	4.70312300	3.30196400	-1.18281800
H	4.89890600	0.99505700	-0.17088100
C	2.94753600	-0.25774100	1.31157600
O	2.09393000	-0.64671700	2.06928200
O	4.03486400	-0.94910400	1.00801000
C	4.15311300	-2.23566600	1.61015100
H	4.07365100	-2.15200400	2.70177500
H	5.13580400	-2.61730700	1.31915100
H	3.36032000	-2.89639500	1.23618300
N	-2.50560600	-0.35949500	1.54568300
C	-3.10962800	0.61671400	0.86645500
C	-3.07549700	-1.55881300	1.54669100
C	-4.29823400	0.44499200	0.15767400
C	-4.26583600	-1.83845000	0.86989800
C	-4.88518600	-0.81823300	0.15879800
H	-4.73314200	1.28380900	-0.38284500
H	-5.80924500	-1.00035300	-0.39119900
H	-2.56151100	-2.34894900	2.09887500
H	-4.68117100	-2.84585000	0.89720900
C	-2.40407500	1.94300600	0.87955900
O	-1.30717900	2.11876200	1.35323400
O	-3.11655500	2.90325600	0.30980300
C	-2.48943800	4.17297300	0.18790500
H	-1.65183200	4.10222800	-0.51998000
H	-2.12110700	4.51419100	1.16393800
H	-3.25263000	4.85504900	-0.19754200

Table S24. Atomic coordinates and single point energies for **42a**.

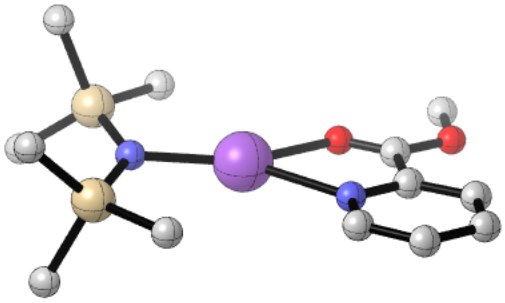


G = –1985.835865
G_{SP} = –1987.50386

N	-2.21117200	0.36116900	-0.29013600
Si	-2.64174700	1.68691100	0.66450800
Si	-3.21444100	-0.62354300	-1.23270100
C	-1.20191800	2.16590800	1.82007700
C	-4.12951100	1.36799200	1.81113100
C	-3.05495500	3.26436400	-0.31136500
C	-4.10133200	-1.99804400	-0.25491700
C	-2.16146400	-1.54132000	-2.53536500
C	-4.57496000	0.28912500	-2.19529300
Na	-0.10719400	-0.07792500	-1.04412200
H	-3.93774100	0.50343200	2.46780400
H	-5.03059600	1.13675300	1.21976800
H	-4.36050800	2.23618500	2.44898900
H	-2.20680300	3.54315200	-0.95711800
H	-3.28313800	4.11738900	0.34785900
H	-3.92453800	3.09607500	-0.96583200
H	-0.92222300	1.31351600	2.46157800
H	-1.46173400	3.01362700	2.47413000
H	-0.31402000	2.45615500	1.23206400
H	-3.37569800	-2.69425000	0.19670700
H	-4.77476400	-2.58839400	-0.89684800
H	-4.70274000	-1.56471600	0.56031500
H	-5.27370200	0.78666300	-1.50295900
H	-5.16096700	-0.39325700	-2.83139200
H	-4.13498800	1.06795700	-2.83781800
H	-1.39651600	-2.17592700	-2.05501500
H	-1.65208700	-0.83408000	-3.21298900

H	-2.77962100	-2.20063000	-3.16425400
N	1.81649900	0.69692100	0.59340500
C	1.81778700	0.48450900	1.90429900
C	2.22609900	1.88576000	0.14675300
C	2.20349300	1.45522100	2.83257700
C	2.61478700	2.92680800	0.98937000
C	2.59241600	2.70417400	2.36517800
H	1.47738300	-0.49964100	2.24181800
H	2.16878700	1.23448900	3.89916100
H	2.86644200	3.50015800	3.05865700
H	2.89655600	3.89687700	0.58001800
C	2.10961200	2.07616900	-1.34989800
O	1.20020200	1.59122200	-1.96371700
O	3.00402300	2.84360300	-1.97288600
C	4.33657500	3.01483500	-1.51675400
H	4.46469100	4.01096900	-1.07230300
H	4.98411000	2.93419600	-2.39775200
H	4.62189300	2.24622900	-0.78607200
N	-0.00986500	-1.89541600	0.50894600
C	1.09964000	-2.62847700	0.50374700
C	-0.82392300	-1.94645700	1.55714500
C	1.46782100	-3.46766700	1.55461700
C	-0.54403100	-2.75788600	2.66432200
C	0.61703700	-3.52592900	2.66015900
H	2.38783800	-4.04765700	1.49801300
H	0.86077000	-4.16790100	3.50816000
H	-1.70792000	-1.30113400	1.48334900
H	-1.23192200	-2.77952600	3.50974800
C	1.93665200	-2.45353300	-0.73321000
O	1.65834000	-1.69228000	-1.62375400
O	3.01764700	-3.22653800	-0.73805500
C	3.84932700	-3.12236600	-1.88735300
H	4.22937700	-2.09751500	-1.99083500
H	3.28253600	-3.37926000	-2.79159400
H	4.67276100	-3.82580500	-1.73483500

Table S25. Atomic coordinates and single point energies for **42b**.

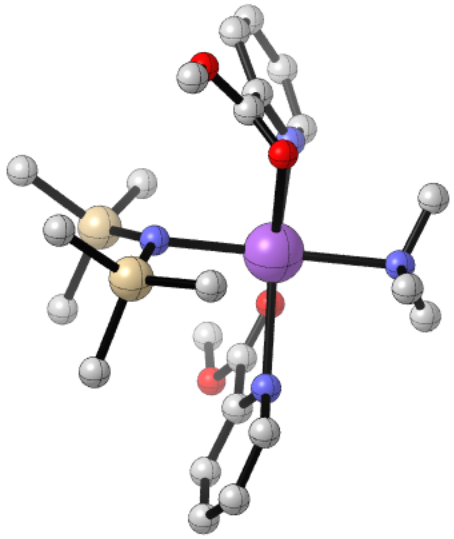


G = –1510.332815
G_{SP} = –1511.466763

N	-2.01408600	0.01250100	-0.02175300
Na	0.16186400	0.27866300	-0.09609500
Si	-2.87623400	1.45634400	0.19178000
C	-1.67339100	2.92321300	-0.00753100
C	-3.65051100	1.65608700	1.91509900
C	-4.28317200	1.72834100	-1.05403900
Si	-2.58589900	-1.57013400	-0.18674700
C	-1.09145600	-2.75804500	-0.07029500
C	-3.40508800	-1.95014700	-1.85733600
C	-3.81816400	-2.12363200	1.14706500
H	-3.91405600	1.63434200	-2.08726900
H	-4.75038900	2.71946500	-0.94067000
H	-5.07033400	0.96969700	-0.91308000
H	-2.87802700	1.57840700	2.69643300
H	-4.38902900	0.86101600	2.10279000
H	-4.15948200	2.62652500	2.02966200
H	-0.87282600	2.88988100	0.75220700
H	-2.18404400	3.89201000	0.10765300
H	-1.20017500	2.91533200	-1.00390600
H	-2.71701500	-1.72055300	-2.68615500
H	-4.30418400	-1.32966000	-1.99618200
H	-3.70567800	-3.00687700	-1.94069200
H	-3.41038500	-1.94404700	2.15407300
H	-4.07282600	-3.19181000	1.05940600
H	-4.75490800	-1.54898900	1.06249900
H	-0.37467000	-2.54209600	-0.88286000
H	-1.37930900	-3.81708400	-0.15952700
H	-0.58249600	-2.62532300	0.90006400
N	2.30262700	-1.00573800	0.06558100
C	2.48692300	-2.31560000	0.20390200
C	3.38016400	-0.21618600	0.02837400

C	3.75734000	-2.89047700	0.31135800
C	4.68655300	-0.68971300	0.12676500
C	4.87379200	-2.06386700	0.27210400
H	1.58593900	-2.93380700	0.22857700
H	3.85449800	-3.97019700	0.42334700
H	5.87910200	-2.47918400	0.35311000
H	5.52122300	0.00839900	0.08923300
O	1.96116800	1.68977100	-0.21714300
O	4.16613800	2.00012800	-0.16453400
C	3.08228800	1.24892100	-0.13028900
C	3.95488200	3.40465000	-0.31300900
H	3.35285100	3.78492800	0.52172500
H	3.42836600	3.60838600	-1.25381500
H	4.94801000	3.86118100	-0.31642700

Table S26. Atomic coordinates and single point energies for **42c**.



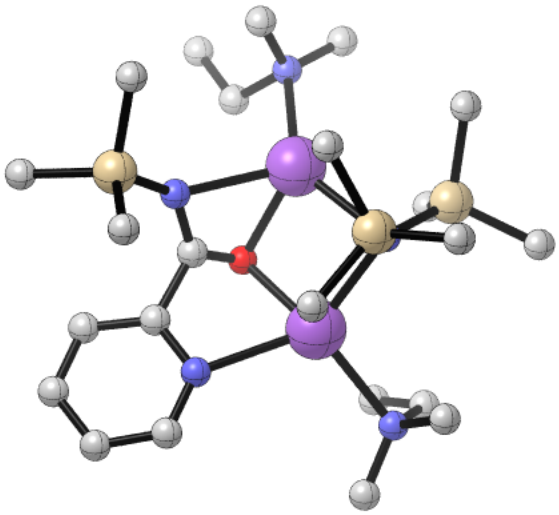
G = –2160.001577
G_{SP} = –2161.864042

N	-0.14901600	-1.39693000	0.07350500
Si	-0.33681400	-1.91310800	1.67768000
Si	0.62218800	-2.30724500	-1.13024300
C	-1.27500900	-0.65565100	2.75298300
C	1.30841100	-2.20408800	2.60745000
C	-1.32041400	-3.53011900	1.87017100
C	-0.18139800	-3.99310700	-1.53477600
C	2.43785900	-2.76598100	-0.73941500
C	0.65866100	-1.36499700	-2.79508300
Na	-0.07711900	0.82819200	-0.58104500
H	1.96151000	-1.31604600	2.57360600
H	1.87342100	-3.03392400	2.15534600
H	1.13371900	-2.45533000	3.66683600
H	-2.29059800	-3.43795200	1.35496400
H	-1.51391500	-3.77048500	2.92804700
H	-0.78813800	-4.38291000	1.42087800
H	-0.85750900	0.35596400	2.64125300
H	-1.22228300	-0.94529700	3.81578300
H	-2.33993400	-0.61465000	2.47500600
H	0.13504200	-4.75348800	-0.80365300
H	0.10794500	-4.35576400	-2.53491300
H	-1.28000600	-3.94312400	-1.48571700
H	-0.32052600	-1.38101800	-3.29511800
H	1.39792600	-1.81426000	-3.47832600

H	0.91882800	-0.30160300	-2.67216900
H	2.46831100	-3.64884600	-0.08081600
H	2.95407600	-1.95162600	-0.20773800
H	3.01382300	-3.01204500	-1.64699400
N	-2.26996300	1.44327300	0.41182300
C	-2.56688800	2.14159400	1.50025100
C	-3.12370300	0.50451100	0.00843000
C	-3.74708900	1.95401000	2.22323700
C	-4.31613300	0.21565700	0.67311900
C	-4.63442900	0.96918100	1.80100900
H	-1.82500400	2.88016800	1.81868000
H	-3.95153500	2.56082100	3.10522200
H	-5.56073000	0.78311500	2.34640600
H	-4.96507200	-0.57544400	0.30130400
C	-2.74755200	-0.19270200	-1.27109900
O	-1.93117000	0.24135300	-2.04582400
O	-3.47414600	-1.27694200	-1.48566000
C	-3.20024600	-1.98517600	-2.68895500
H	-3.89710700	-2.82799800	-2.71211900
H	-2.16463100	-2.34577600	-2.68052700
H	-3.35154300	-1.33072700	-3.55798900
N	2.53580400	0.80986600	-0.71307700
C	2.98315900	0.77438300	0.54384000
C	3.36338500	0.42150200	-1.67737600
C	4.26521200	0.34708400	0.89264900
C	4.67175100	-0.00644000	-1.43827200
C	5.12833000	-0.04784600	-0.12691600
H	4.56176700	0.32741300	1.93953500
H	6.13779800	-0.39009300	0.10399200
H	2.97122700	0.43629300	-2.69779900
H	5.30395500	-0.31305700	-2.27133000
C	2.01733700	1.24600200	1.59741600
O	0.91465600	1.67514300	1.36499000
O	2.52748400	1.15182300	2.81787400
C	1.65789200	1.46278600	3.90110700
H	0.86068800	0.70971600	3.96020000
H	1.21317400	2.45642500	3.76100300
H	2.27570400	1.43837800	4.80327500
N	-0.00358900	2.95385300	-1.79726400
C	0.43955200	2.53590300	-3.11384000
C	0.94375200	3.86117600	-1.17995800
C	-1.33152500	3.53481800	-1.86126600
H	-0.25612200	1.78638400	-3.51826600
H	1.43833800	2.08152400	-3.03907300

H	0.50058900	3.38773800	-3.82519000
H	1.05998200	4.80269600	-1.75881700
H	1.92507500	3.37208000	-1.10115600
H	0.60790500	4.11361000	-0.16411400
H	-2.03985100	2.78714900	-2.24357000
H	-1.35757100	4.43094700	-2.51801500
H	-1.65838100	3.82942600	-0.85473800

Table S27. Atomic coordinates and single point energies for **46**.



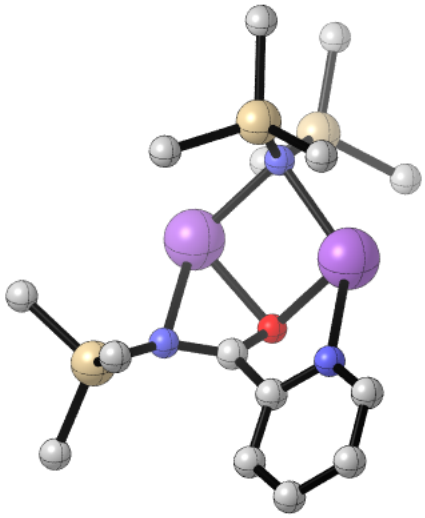
G = –2448.082940
G_{SP} = –2449.915069

C	0.74970700	4.26774500	-0.45014900
C	1.92166200	4.96381700	-0.74114000
C	3.04992100	4.23073500	-1.10255300
C	2.97044800	2.84167900	-1.12424900
C	1.75647400	2.23267700	-0.80016600
N	0.66026400	2.93952900	-0.49662000
H	-0.16029100	4.80784100	-0.17304400
H	3.98156900	4.73622900	-1.36286200
H	1.93957200	6.05250800	-0.69579500
H	3.82467600	2.22405300	-1.39761400
C	1.57431600	0.72061000	-0.77852000
N	2.32243400	-0.05497800	-0.04025800
O	0.58705100	0.32208700	-1.46535000
Si	3.57195000	0.27039300	1.12749300
C	3.96659900	-1.35486600	1.99537500
C	3.02469800	1.53253600	2.41985300
C	5.21738600	0.84123500	0.37745200
H	2.16765600	1.15245200	2.99650900
H	2.72375600	2.48513600	1.95499500
H	3.84320800	1.74298900	3.12592700
H	5.39470400	0.36366600	-0.59898500
H	6.04120700	0.54721600	1.04634600
H	5.27247000	1.93153900	0.24838700
H	3.07109100	-1.83555600	2.41599800
H	4.67491000	-1.18150400	2.82041800

H	4.44031700	-2.06006300	1.29455700
Na	-1.18531400	1.27293600	-0.42972500
Na	0.35530100	-1.50186800	-0.14815400
N	-1.71106800	-0.67039100	0.73095500
Si	-2.68630700	-1.94721700	0.16522400
C	-2.21483000	-3.61297000	0.96258700
C	-2.42367100	-2.15835100	-1.70675200
C	-4.55430200	-1.75742800	0.44365400
Si	-1.37936900	-0.27279300	2.35566200
C	-0.79972900	1.53603600	2.46131600
C	0.07535800	-1.29358800	3.03736300
C	-2.82950900	-0.47806600	3.55807600
H	-1.35732300	-2.28587500	-1.95848100
H	-2.77351000	-1.27418700	-2.26302300
H	-2.96537100	-3.03479600	-2.09617600
H	-1.13067000	-3.79948800	0.87064100
H	-2.74267700	-4.46546900	0.50617800
H	-2.44976500	-3.60804200	2.03947800
H	-4.77183700	-1.58883400	1.50981700
H	-5.08866900	-2.66795400	0.12931900
H	-4.97942900	-0.91281300	-0.12055200
H	-3.68812200	0.13873400	3.24850200
H	-2.54925600	-0.18147500	4.58084900
H	-3.16767200	-1.52604400	3.59313600
H	0.97999600	-1.09039000	2.43778100
H	-0.13831200	-2.37376400	2.98274800
H	0.31943000	-1.04893200	4.08323100
H	0.11072700	1.69192800	1.85797300
H	-0.55041900	1.81802400	3.49629700
H	-1.56885500	2.24315500	2.10612700
N	-3.28735100	2.38648900	-0.74766500
C	-4.06576500	2.14180600	0.45982000
C	-3.27905800	3.79881600	-1.08796400
C	-3.79058700	1.55155700	-1.83901500
C	-2.92470500	1.56635100	-3.09114400
H	-4.82994600	1.85066400	-2.09697800
H	-3.84772100	0.52282200	-1.45005600
H	-2.90092700	2.55463900	-3.57056700
H	-3.33056600	0.85661800	-3.82501100
H	-1.88643100	1.26012500	-2.88346100
H	-4.29118600	4.16803900	-1.35626400
H	-2.60330700	3.99226400	-1.93191400
H	-2.92054100	4.38042900	-0.22689600
H	-3.94459500	1.09235700	0.76759500

H	-5.14396100	2.35314600	0.30442200
H	-3.70498800	2.78468600	1.27505900
N	1.17301800	-3.50297900	-1.20638800
C	0.35824400	-4.60831000	-1.68216500
C	2.03977200	-3.91226200	-0.11148800
C	1.89706700	-2.81409700	-2.28322300
C	2.89996900	-3.66118800	-3.06522600
H	-0.31140300	-4.95232100	-0.88058000
H	0.96524700	-5.47366300	-2.01402200
H	-0.26398700	-4.27720400	-2.52577500
H	2.63381000	-3.05089400	0.22898600
H	2.73434000	-4.73058500	-0.38622100
H	1.42771500	-4.26807200	0.73251600
H	3.68982200	-4.06556700	-2.41544100
H	3.38813600	-3.04026600	-3.82902400
H	2.41658300	-4.50257100	-3.58244100
H	2.40731000	-1.94851100	-1.83032700
H	1.14152500	-2.40077300	-2.97075200

Table S28. Atomic coordinates and single point energies for **46a**.

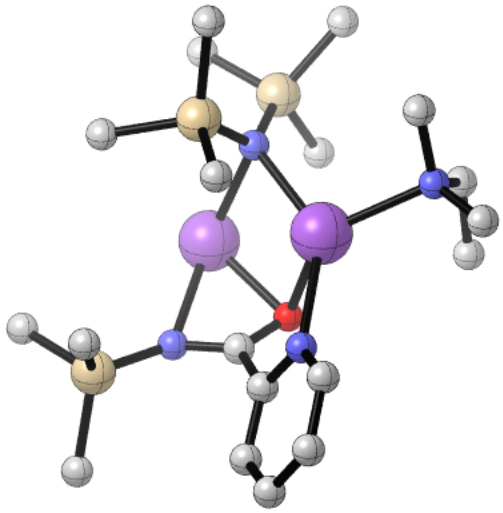


G = –2021.299996
G_{SP} = –2022.650064

C	2.12475100	3.21723500	0.84763100
C	3.50703200	3.37711500	0.78207400
C	4.23991400	2.46789000	0.02236200
C	3.56852600	1.42720200	-0.61101300
C	2.18047600	1.34579500	-0.48777100
N	1.47219000	2.24230200	0.21362700
H	1.51619700	3.91210200	1.43356300
H	3.98947600	4.20019300	1.30858500
H	5.32281400	2.56643100	-0.07015800
H	4.09709800	0.68263600	-1.20564500
C	1.36351800	0.24241500	-1.14700600
O	0.33566900	0.66509500	-1.75858700
N	1.65861700	-1.01661300	-0.99784500
Si	2.86851600	-1.94371900	-0.16487600
C	2.13460500	-3.66204600	0.06948500
C	3.33348500	-1.26893500	1.53822700
C	4.42718600	-2.15352700	-1.21122600
H	2.43458400	-1.12988100	2.15863200
H	3.86212200	-0.30629800	1.48753500
H	3.98821700	-1.98771500	2.05573000
H	4.15648400	-2.42808500	-2.24178900
H	5.04899600	-2.96236500	-0.79721000
H	5.05221500	-1.24969400	-1.25338900
H	1.22864200	-3.62512300	0.69323400
H	2.85092300	-4.34109200	0.55654600

H	1.86565900	-4.09581200	-0.90621300
Na	-0.87890700	1.76774900	-0.28057400
Na	-0.68952400	-1.29707900	-1.23596200
N	-2.22204900	-0.11999300	0.06690400
Si	-2.04441900	-0.45880700	1.72460000
C	-1.32729800	1.05497100	2.64044900
C	-0.75577600	-1.83451100	1.94703300
C	-3.60584700	-0.97678000	2.65608300
Si	-3.52576000	0.18805600	-0.97698000
C	-3.47468600	1.99922000	-1.58628600
C	-5.26194600	-0.10442200	-0.29132600
C	-3.35186500	-0.86091800	-2.55761000
H	-4.36290500	-0.17817600	2.65411000
H	-3.36914200	-1.21674200	3.70450600
H	-4.05982500	-1.86928900	2.19868100
H	-0.31614200	1.30578900	2.27257000
H	-1.23283200	0.87605500	3.72275100
H	-1.97752600	1.93787900	2.51188700
H	0.17936100	-1.55295600	1.43278500
H	-1.11348700	-2.78422100	1.51408900
H	-0.50745600	-2.02510000	3.00263200
H	-5.47642500	0.57171700	0.55035400
H	-5.37847500	-1.13661800	0.07201400
H	-6.02173400	0.07189300	-1.06868000
H	-3.51219000	2.70524600	-0.73785000
H	-4.32878700	2.23964900	-2.23782700
H	-2.56661700	2.20031000	-2.18258000
H	-2.42637300	-0.60819300	-3.10459400
H	-4.18332800	-0.69404300	-3.25934100
H	-3.34263100	-1.93813800	-2.31821100

Table S29. Atomic coordinates and single point energies for **46b**.



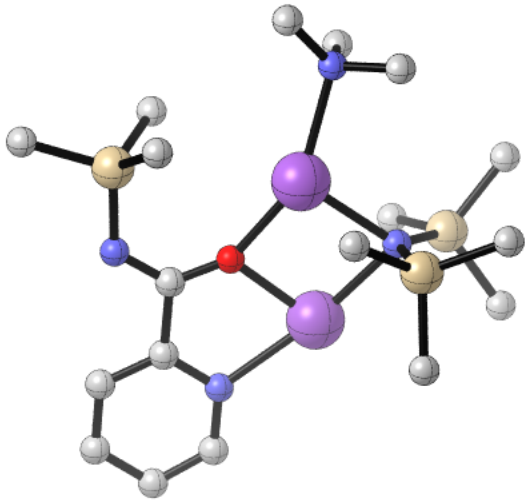
G = –2234.690219
G_{SP} = –2236.281216

C	2.20629400	3.03500100	1.08351600
C	3.54403700	3.40893700	0.96712700
C	4.34797600	2.70983500	0.06918500
C	3.79419600	1.65358800	-0.64797600
C	2.44606300	1.34643300	-0.45474300
N	1.66389800	2.04321000	0.37909300
H	1.54128100	3.56301700	1.77324100
H	5.39542000	2.98375900	-0.06849500
H	3.93722700	4.23408200	1.56056000
H	4.38100200	1.07320000	-1.35890100
C	1.75114700	0.19883900	-1.17127300
N	2.19358100	-1.02591300	-1.10255900
O	0.66622300	0.53279300	-1.73839100
Si	3.48954500	-1.79462300	-0.23115600
C	3.20194600	-3.64729400	-0.39919000
C	3.48911400	-1.32608000	1.59759100
C	5.20688400	-1.45668700	-0.95363800
H	2.55327200	-1.64406000	2.08245600
H	3.59072200	-0.23789600	1.73694400
H	4.32458000	-1.81412200	2.12345900
H	5.16222600	-1.36927000	-2.05023300
H	5.87837400	-2.29511400	-0.71197100
H	5.66491300	-0.54285900	-0.54864000
H	2.22166900	-3.94859400	-0.00049000
H	3.97264000	-4.22016700	0.13874500

H	3.24146500	-3.93827800	-1.46035000
Na	-0.62345900	1.13162700	0.00518900
Na	-0.06800700	-1.58162500	-1.48214600
N	-1.72137700	-0.95428700	0.07051600
Si	-3.09770800	-1.44319500	-0.81403600
C	-3.35159700	-3.32832200	-0.81355900
C	-2.85141700	-0.96545800	-2.64352900
C	-4.76087900	-0.70959800	-0.26670500
Si	-1.34344600	-1.44904100	1.66329400
C	-0.20305600	-0.15817600	2.47669000
C	-0.35656000	-3.06997000	1.69201700
C	-2.83337900	-1.66514500	2.81472200
H	-2.12050000	-1.61596600	-3.15723100
H	-2.49455600	0.07202300	-2.74939900
H	-3.79049400	-1.06130800	-3.21019800
H	-2.45161400	-3.85058700	-1.18014700
H	-4.19529800	-3.62968800	-1.45421200
H	-3.55196000	-3.70356200	0.20289700
H	-4.92744100	-0.88836700	0.80706100
H	-5.58509000	-1.18838900	-0.81868900
H	-4.83351100	0.37455600	-0.44065700
H	-3.39436900	-0.72221800	2.91390600
H	-2.51689500	-1.97793900	3.82195600
H	-3.52876300	-2.42810700	2.43020200
H	0.57323600	-2.94962500	1.10995000
H	-0.93430800	-3.89350000	1.24292000
H	-0.06850200	-3.37302000	2.71089800
H	0.72589400	-0.01777800	1.89752900
H	0.09696500	-0.48310200	3.48505500
H	-0.69033800	0.82665700	2.59037300
N	-2.23848400	2.83901900	0.32303600
C	-3.14250200	2.32755700	1.34406900
C	-1.81544200	4.19545500	0.62504700
C	-2.85409400	2.72332100	-1.00082500
C	-1.92087700	3.05615900	-2.15732200
H	-3.76421400	3.36001200	-1.05206900
H	-3.19571300	1.68076400	-1.10183800
H	-1.62886400	4.11539100	-2.16397400
H	-2.43505700	2.85492000	-3.10723800
H	-1.00429900	2.44332700	-2.14393100
H	-2.66115600	4.91352800	0.58495200
H	-1.04238200	4.52703900	-0.08064000
H	-1.38642200	4.22831200	1.63651100
H	-3.34706600	1.26271100	1.15630700

H	-4.10572100	2.87834800	1.35957200
H	-2.67792800	2.42097300	2.33620200

Table S30. Atomic coordinates and single point energies for **46d**.

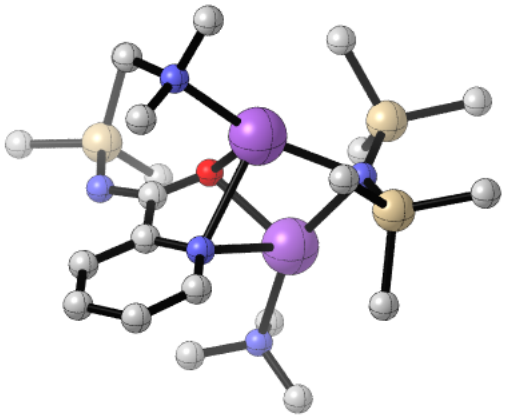


G = –2195.455306
G_{SP} = –2197.002290

N	1.93907500	-0.85240600	0.01271900
N	-3.39490200	0.88025800	-0.00206400
Na	-0.11873500	-1.90794800	-0.31606100
Na	0.55912600	1.01956500	0.04320000
Si	2.26843200	-1.06203200	1.67668000
C	1.24307800	0.20030900	2.66986100
C	4.08241400	-0.87103500	2.18384300
C	1.69884700	-2.76467100	2.30859300
Si	2.91832900	-1.34086200	-1.29783900
C	4.51074300	-0.33916600	-1.54538500
C	1.91238000	-1.18981500	-2.90473900
C	3.45910000	-3.15907800	-1.18073900
Si	-2.84688300	2.52687500	0.01293100
C	-4.35861000	3.64073200	0.05627200
C	-1.86337600	2.94427400	-1.55290900
C	-1.80637200	2.93347000	1.54430500
H	0.60673700	-2.89288100	2.20478800
H	1.93187900	-2.90628100	3.37548000
H	2.19240600	-3.57359500	1.74657100
H	4.47068800	0.12519200	1.92100700
H	4.71160600	-1.61874800	1.67507900
H	4.20944400	-1.00912600	3.26879400
H	1.52696600	1.24402600	2.44833600
H	1.37465700	0.06135600	3.75362300
H	0.16549800	0.08150900	2.45903500

H	4.03780300	-3.47512300	-2.06273100
H	2.58630700	-3.82829200	-1.09666900
H	4.08662400	-3.32754900	-0.29059000
H	4.31023100	0.70628400	-1.82632200
H	5.12771700	-0.78252400	-2.34270700
H	5.11112300	-0.32777100	-0.62223700
H	2.52617800	-1.41388100	-3.79078500
H	1.50246200	-0.17414200	-3.03101700
H	1.05844600	-1.88943600	-2.92603300
H	-2.36691400	2.65332700	2.44925800
H	-1.59717500	4.01337100	1.59995300
H	-0.84392500	2.40062200	1.59326200
H	-2.49021900	2.75654800	-2.43792800
H	-0.96823100	2.31236000	-1.66174400
H	-1.55751800	4.00227300	-1.57734000
H	-5.00095400	3.44626200	-0.81552500
H	-4.08436800	4.70654000	0.05328300
H	-4.95419200	3.44028800	0.95949100
N	-2.39182300	-2.57087000	-0.21915000
C	-2.93643300	-3.79064500	-0.24886400
C	-3.19979100	-1.50632600	-0.11227100
C	-4.30639800	-4.01684500	-0.17484600
C	-4.59083000	-1.64074700	-0.03416000
C	-5.14995800	-2.91120200	-0.06528000
H	-2.24508000	-4.63431100	-0.33562400
H	-4.69646000	-5.03415200	-0.20275500
H	-6.23174100	-3.04277300	-0.00488400
H	-5.17823200	-0.72748200	0.04843300
O	-1.29160800	-0.07999200	-0.12641100
C	-2.57393100	-0.10966000	-0.07664600
N	1.90225900	2.98458400	-0.19118900
C	3.15795900	2.65762700	0.47301000
C	2.08075500	2.97025800	-1.63705600
H	2.41256100	1.97210000	-1.96145500
H	1.13128900	3.20763800	-2.13785100
H	2.84126900	3.70774300	-1.96583500
C	1.38364100	4.26727100	0.25790600
H	0.41743200	4.46887900	-0.22608700
H	1.22486200	4.24645100	1.34533200
H	2.07834800	5.09856800	0.01979800
H	3.02871700	2.69754600	1.56371500
H	3.96357100	3.36720400	0.19385500
H	3.46889200	1.63893500	0.19738300

Table S31. Atomic coordinates and single point energies for **46e**.



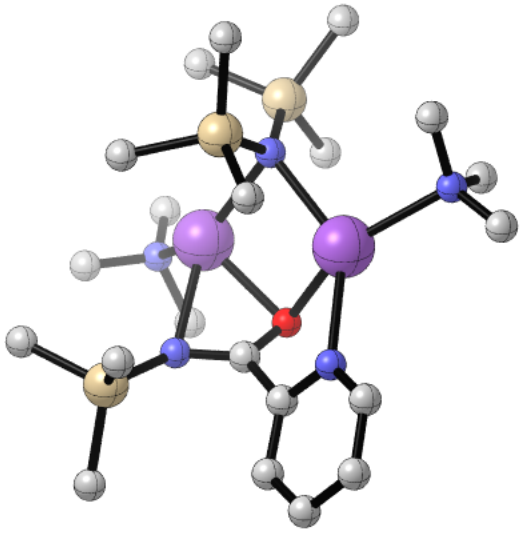
G = –2369.611915
G_{SP} = –2371.356254

N	2.39763900	-0.43764000	-0.60717500
N	-3.21263600	0.15434400	-0.00306200
Na	0.60050900	-1.41915600	0.44382000
Na	0.75564800	1.21213900	-0.55004400
Si	3.57269100	0.04678800	0.50949700
C	3.35560200	1.89966800	0.93091700
C	5.38022400	-0.15884200	-0.00663100
C	3.35911700	-0.91317100	2.14167800
Si	2.34160900	-0.91377400	-2.23727800
C	1.62451400	0.49439600	-3.31049100
C	1.12134800	-2.35741900	-2.42930900
C	3.98662700	-1.42681500	-3.01470200
Si	-3.88368200	-0.43860200	-1.50472400
C	-3.45390500	-2.25761100	-1.76732600
C	-3.26635600	0.56113500	-2.98054300
C	-5.75295300	-0.26631500	-1.38352600
H	2.31876900	-0.86739100	2.50844000
H	4.00897500	-0.53874900	2.94823000
H	3.60630700	-1.97521800	1.97918400
H	5.61556700	0.46922600	-0.87967900
H	5.59688300	-1.20311600	-0.27884600
H	6.06002700	0.12946000	0.81054300
H	3.52861500	2.50047800	0.02151500
H	4.06179300	2.25148800	1.69924900
H	2.33834300	2.12425800	1.29793500
H	3.84451500	-1.74681500	-4.05873100
H	4.43590300	-2.26520000	-2.46022400

H	4.70926100	-0.59675300	-3.00858700
H	0.57215300	0.69909600	-3.04140500
H	1.62775300	0.24908600	-4.38365200
H	2.21331500	1.41841500	-3.17914200
H	1.02926400	-2.69804000	-3.47196900
H	0.11748200	-2.03775900	-2.09885400
H	1.44208100	-3.22369000	-1.82582300
H	-6.13978600	-0.84750400	-0.53289700
H	-6.25299000	-0.62016300	-2.29784600
H	-6.03324900	0.78582400	-1.22392200
H	-2.17082000	0.48032700	-3.04360000
H	-3.53788900	1.62304700	-2.87683700
H	-3.69921400	0.19214400	-3.92309500
H	-2.36659200	-2.36615000	-1.89576700
H	-3.95048900	-2.66459600	-2.66156100
H	-3.77104700	-2.86007500	-0.90152200
N	-0.15066300	0.66789000	1.79964900
C	0.28563200	1.12701100	2.97789600
C	-1.46532700	0.70316700	1.54139400
C	-0.56318700	1.64168700	3.95310300
C	-2.39246400	1.20344100	2.46374400
C	-1.93353100	1.67902100	3.68542600
H	1.36557800	1.08209200	3.14844400
H	-0.15584800	2.00335000	4.89710600
H	-2.63156500	2.07545400	4.42504200
H	-3.44302800	1.18953700	2.17522700
O	-0.99581000	-0.21893200	-0.59744200
C	-1.93698100	0.16126300	0.18563400
N	-0.11224400	3.43071500	-0.50825800
C	0.77871200	4.22250500	-1.34430000
C	-1.42309800	3.29046000	-1.13252200
H	-1.32335300	2.79237000	-2.10805900
H	-2.08365500	2.67267100	-0.50624200
H	-1.90722600	4.27590000	-1.29119300
C	-0.22513500	4.01284800	0.82052500
H	-0.89065700	3.39970500	1.44515900
H	0.76479000	4.05367900	1.29844500
H	-0.63655700	5.04259200	0.78177200
H	1.77331400	4.28431700	-0.87942900
H	0.39789800	5.25403300	-1.49094600
H	0.88372700	3.75331300	-2.33362100
N	-0.50550800	-3.08020000	1.75924700
C	-0.93380200	-4.01883800	0.73012300
H	-1.55431900	-3.49941600	-0.01402700

H	-0.05824000	-4.44341000	0.21765100
H	-1.52473000	-4.85551000	1.15569800
C	0.37568800	-3.72285600	2.72168100
H	1.26199100	-4.12744300	2.21181800
H	0.71265900	-2.99072200	3.46921200
H	-0.13064200	-4.55531400	3.25210900
C	-1.65886200	-2.48758400	2.42420100
H	-1.32562600	-1.73588300	3.15548700
H	-2.30963500	-1.99059700	1.68896700
H	-2.25699800	-3.25415500	2.95867100

Table S32. Atomic coordinates and single point energies for **46f**.



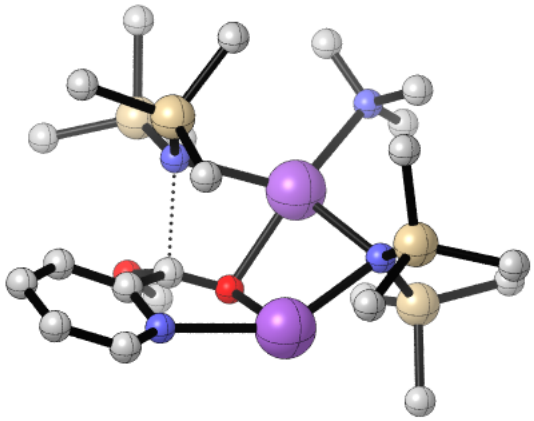
G = –2369.607022
G_{SP} = –2371.352467

C	2.03885700	3.75907900	-0.50989800
C	3.37882500	4.05693300	-0.75168700
C	4.23029900	3.01420500	-1.11018600
C	3.71869300	1.72192200	-1.17600000
C	2.36545000	1.51880300	-0.89809200
N	1.53736700	2.52823500	-0.59974600
H	1.33681900	4.55259600	-0.23791400
H	5.28120000	3.20609000	-1.33381500
H	3.73634100	5.08332100	-0.67193600
H	4.34353000	0.87286700	-1.44892100
C	1.72060200	0.13880000	-0.92610600
N	2.18299600	-0.85519000	-0.21479200
O	0.66744200	0.08817700	-1.62730700
Si	3.45078400	-0.97288000	0.97230000
C	3.29026000	-2.65496400	1.80711800
C	3.31680200	0.36812500	2.29437200
C	5.20445600	-0.94616600	0.25108200
H	2.37687100	0.26595900	2.85806800
H	3.33967800	1.37837700	1.85541100
H	4.15122100	0.28946600	3.00882900
H	5.23199200	-1.42466000	-0.74047300
H	5.87694400	-1.51347700	0.91322200
H	5.61405100	0.06996200	0.16030300
H	2.27426600	-2.84285100	2.18458400

H	3.98379300	-2.71912800	2.66006800
H	3.55293500	-3.46274600	1.10641500
Na	-0.75054000	1.53115100	-0.62417700
Na	-0.14046000	-1.59919300	-0.35081400
N	-1.87498200	-0.17512600	0.48304900
Si	-3.18231300	-1.06178000	-0.15281400
C	-3.27865000	-2.82053000	0.57384400
C	-2.94611700	-1.27477600	-2.02823500
C	-4.90214000	-0.30030200	0.10319600
Si	-1.46461400	0.04528700	2.12261200
C	-0.33057300	1.56275900	2.29476600
C	-0.42160600	-1.40740100	2.77821200
C	-2.92526500	0.26850200	3.30920500
H	-1.95373000	-1.69331400	-2.26633800
H	-3.01372200	-0.31112000	-2.55758600
H	-3.70634400	-1.94524400	-2.45926600
H	-2.31107100	-3.34204700	0.47197600
H	-4.04592900	-3.43888400	0.08147500
H	-3.51405300	-2.78310700	1.64998800
H	-5.08336100	-0.10110000	1.17102900
H	-5.68955400	-0.98355600	-0.25227600
H	-5.02073700	0.65133800	-0.43822700
H	-3.54088600	1.13614500	3.02402800
H	-2.58271800	0.42068300	4.34459900
H	-3.57701300	-0.61988700	3.29842900
H	0.52374600	-1.46922500	2.21076500
H	-0.95569000	-2.36528800	2.66466100
H	-0.15082400	-1.29515400	3.83994400
H	0.59640200	1.41871600	1.71375800
H	-0.03121000	1.72594800	3.34197900
H	-0.80951500	2.49150000	1.94110400
N	-2.39071200	3.30598100	-0.70192900
C	-3.24033700	3.19288800	0.47562500
C	-1.92362700	4.66685800	-0.89458500
H	-2.76075400	5.37519500	-1.06569500
H	-1.24935900	4.71521000	-1.76225700
H	-1.37013800	4.99919300	-0.00460600
H	-3.46979800	2.13330900	0.66029900
H	-4.18832200	3.75654700	0.35179600
H	-2.71658800	3.59053400	1.35613900
N	0.05198100	-3.68743900	-1.51456500
C	-1.03269600	-4.52153700	-2.00266000
C	0.86993800	-4.40259500	-0.54663200
H	-1.65852700	-4.85964300	-1.16496700

H	-0.65016800	-5.41638100	-2.53645300
H	-1.66608200	-3.94918400	-2.69453000
H	1.66562200	-3.73928400	-0.17792300
H	1.34232800	-5.30506900	-0.98748600
H	0.25260000	-4.72016900	0.30742800
C	-3.09117500	2.81555300	-1.87871800
H	-2.42853300	2.84131100	-2.75710600
H	-3.40837300	1.77622200	-1.70930500
H	-3.99385200	3.41887800	-2.10788700
C	0.87095800	-3.19322900	-2.61545200
H	0.25242400	-2.59756000	-3.30162400
H	1.66503500	-2.54304000	-2.22014300
H	1.33225300	-4.02677200	-3.18469400

Table S33. Atomic coordinates and single point energies for **TS-1**.



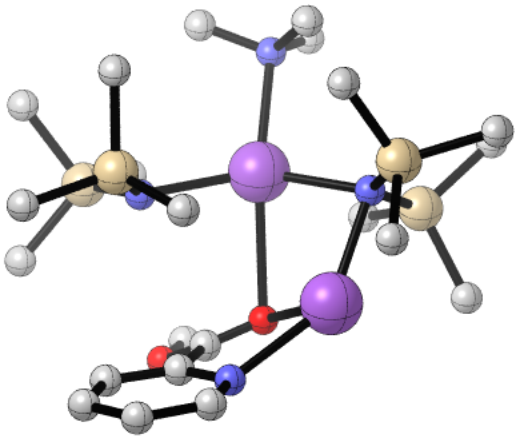
G = –2719.294899
G_{SP} = –2721.216825

N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	4.48057353
Na	2.14401756	0.00000000	0.93273590
Na	-0.71140134	-0.54582211	2.21231036
Si	0.04243108	1.54102079	-0.73719134
C	-1.06152961	2.82233728	0.11319903
C	-0.41714102	1.59690030	-2.57505765
C	1.82788345	2.25379549	-0.66579898
Si	-0.05178624	-1.50113790	-0.81863387
C	-1.41219125	-1.69830636	-2.12766600
C	-0.24614625	-2.94663854	0.40443691
C	1.58674194	-1.87650422	-1.72562117
Si	-0.76218825	-0.89130381	5.75247173
C	-1.43361621	-2.57857278	5.16109701
C	-2.27758192	-0.03668484	6.52858248
C	0.35769455	-1.22342853	7.25048011
Si	-0.06112568	1.72648751	4.53117226
C	0.46653038	2.51520899	6.17593504
C	-1.78704277	2.42234839	4.14293008
C	1.04475666	2.51763665	3.20544512
H	2.17865353	2.46045152	0.36165606
H	1.88385247	3.21466483	-1.20029145
H	2.54661109	1.57828722	-1.16544391
H	-1.46054712	1.28059362	-2.72844004
H	0.22581027	0.93948879	-3.18164573
H	-0.31570065	2.62195633	-2.96495543
H	-2.11754470	2.65785536	-0.15126873

H	-0.79606193	3.84246573	-0.20632818
H	-0.97384822	2.78106500	1.20967976
H	1.54314593	-2.82861902	-2.27758912
H	2.43497620	-1.96222594	-1.02210354
H	1.82841766	-1.08140044	-2.44971106
H	-2.40073765	-1.39269945	-1.75062544
H	-1.48377500	-2.74982703	-2.44798078
H	-1.19888726	-1.09107143	-3.01941929
H	-0.42430293	-3.88410122	-0.14545887
H	-1.08855333	-2.82106592	1.10398395
H	0.66658403	-3.06674162	1.00556110
H	1.23889701	-1.82330949	6.98231958
H	-0.20040475	-1.76321693	8.03189808
H	0.69960917	-0.27161794	7.68950189
H	-3.10617292	0.08819978	5.81687864
H	-2.04380074	0.95213027	6.95060859
H	-2.64151008	-0.66997973	7.35378285
H	-2.43128063	-2.75082270	5.59506459
H	-0.79853292	-3.41770226	5.47786697
H	-1.53851448	-2.62980829	4.06373977
H	2.09164293	2.60900560	3.52712053
H	0.67624002	3.53064873	2.98016384
H	1.01324057	1.94832461	2.26180312
H	-2.54604388	2.10655449	4.87245138
H	-2.12408395	2.10431701	3.14264513
H	-1.75847243	3.52378020	4.13846856
H	-0.17587003	2.19914662	7.01167966
H	0.40779757	3.61306208	6.10621742
H	1.50355099	2.25161929	6.43279841
N	3.41922232	0.44961959	2.94116740
C	4.38962373	1.34565801	3.14216974
C	2.79218612	-0.05600800	4.00510973
C	4.77676628	1.77025475	4.40847345
C	3.11393887	0.29788302	5.31641003
C	4.12109377	1.23218642	5.51746732
H	4.87723172	1.74764203	2.24967381
H	5.57289328	2.50592494	4.52003983
H	4.39251096	1.54293687	6.52761360
H	2.55510463	-0.15016921	6.13784755
O	1.43548737	-1.35686666	2.53158064
C	1.76893712	-1.12677648	3.69586519
O	1.81237082	-2.11608883	4.60314193
C	1.51490295	-3.41673593	4.11734181
H	1.50825373	-4.07384202	4.99344514

H	2.29313882	-3.73813686	3.40956774
H	0.54336570	-3.44904551	3.61176516
N	-3.15962684	-0.90301882	1.90094817
C	-3.40340783	0.19039451	0.96930638
C	-3.62245431	-2.15908559	1.33221866
H	-3.13290336	-2.33810974	0.36508338
H	-3.37920468	-2.99327539	2.00659734
H	-4.72049951	-2.15053526	1.17066895
C	-3.82436655	-0.64727509	3.17022010
H	-3.61852661	-1.46396472	3.87568085
H	-3.44823096	0.28799840	3.60669305
H	-4.92391017	-0.55902938	3.04562002
H	-3.07790858	1.14093599	1.41523081
H	-4.48010906	0.27854122	0.71485312
H	-2.81928013	0.03699836	0.05112881

Table S34. Atomic coordinates and single point energies for **45**.



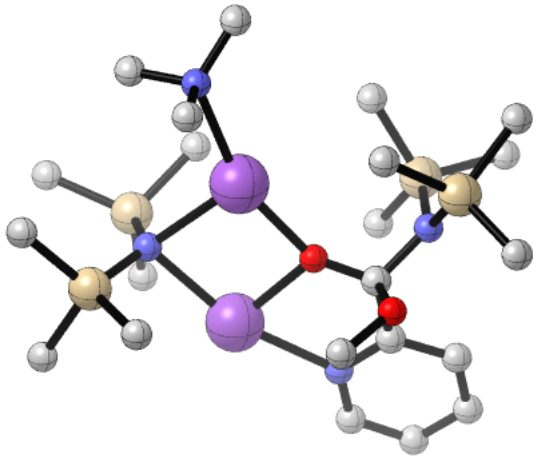
G = –2719.305439
G_{SP} = –2721.231429

N	2.43456200	-0.48324500	0.00681000
N	-1.70902300	0.93845200	0.29081600
Na	1.09641300	-2.27730500	-0.60743700
Na	0.55258300	0.96561300	-0.19610500
Si	3.10433200	-1.19278100	1.41086300
C	2.57785900	-0.38316300	3.03846100
C	4.99545100	-1.29392600	1.46470700
C	2.52982100	-3.02588900	1.55960500
Si	3.25062700	-0.09033800	-1.44406800
C	4.93011000	0.77078900	-1.26922500
C	2.17866400	1.04524600	-2.53289800
C	3.55114100	-1.64146700	-2.51674900
Si	-2.72538200	2.15386700	-0.33990100
C	-1.86270700	3.19127900	-1.70810400
C	-3.34695600	3.44556500	0.91738400
C	-4.33630600	1.48091700	-1.10398600
Si	-1.94906700	0.31164300	1.85755300
C	-3.74608400	-0.13792600	2.29881000
C	-1.37715700	1.46008200	3.26546900
C	-0.94282300	-1.28862400	2.10662500
H	1.43932500	-3.13062900	1.70720600
H	2.99790300	-3.49750800	2.43718400
H	2.84199100	-3.62890800	0.68641100
H	5.44576500	-0.28946600	1.46585700
H	5.40242900	-1.84408700	0.60134100
H	5.32345000	-1.81075300	2.38035000
H	3.12996100	0.55366000	3.20831100

H	2.79704200	-1.05272800	3.88521100
H	1.50108100	-0.15568200	3.06065600
H	4.13386100	-1.41501600	-3.42327700
H	2.59942900	-2.08545000	-2.86089800
H	4.10507400	-2.40820700	-1.94962200
H	4.87904600	1.61952300	-0.56870800
H	5.26081300	1.15854100	-2.24574400
H	5.70563400	0.08397100	-0.90093400
H	2.71460600	1.28985000	-3.46306800
H	1.93592500	2.00222200	-2.04427700
H	1.24023200	0.54246200	-2.81256600
H	-4.14830600	0.74752600	-1.90261100
H	-4.95512300	2.29215500	-1.52007800
H	-4.92843000	0.97861500	-0.32100300
H	-2.52120400	4.01158400	1.37530200
H	-3.91980700	2.97679100	1.73301200
H	-4.01255000	4.16871100	0.41877900
H	-1.94106500	4.26516800	-1.47558100
H	-2.32638900	3.05024200	-2.69633700
H	-0.78774100	2.95625100	-1.80243900
H	-1.50476300	-2.17019000	1.76630300
H	-0.68968100	-1.44729300	3.16677700
H	0.00875200	-1.23685700	1.54937400
H	-1.88022400	2.43827000	3.21487600
H	-0.29026500	1.64015100	3.22249500
H	-1.59684900	1.01675600	4.25003200
H	-4.38276800	0.75967300	2.34438900
H	-3.79674100	-0.63263300	3.28217300
H	-4.18777800	-0.81720200	1.55366500
N	-1.11629700	-3.29083300	-0.56163200
C	-1.55833800	-4.28663700	0.20280600
C	-1.99416300	-2.36330300	-0.95583300
C	-2.88706100	-4.38718400	0.61872100
C	-3.33790000	-2.36590700	-0.59168300
C	-3.78757200	-3.40177500	0.22422500
H	-0.82179500	-5.03293900	0.51215200
H	-3.19774100	-5.21790800	1.25194200
H	-4.82752600	-3.43467900	0.55177900
H	-3.98664400	-1.55661200	-0.92780500
O	-0.24275100	-1.07501100	-1.94025200
C	-1.43271200	-1.29776400	-1.85016900
O	-2.34131900	-0.71967800	-2.59535500
C	-1.87062600	0.28034400	-3.49599600
H	-2.76056800	0.71556600	-3.95966400

H	-1.21910200	-0.17864100	-4.25187100
H	-1.31228500	1.04473700	-2.94357900
N	1.46722700	3.22039800	0.40103600
C	2.30826200	2.72607600	1.47994800
C	2.23914900	4.05252000	-0.50526300
H	3.10136000	3.49021600	-0.89115400
H	1.61574700	4.36314600	-1.35648400
H	2.61931100	4.96492800	-0.00001100
C	0.33600100	3.96047100	0.94117100
H	-0.28883600	4.33923500	0.12194000
H	-0.28332400	3.29728000	1.56069200
H	0.66887800	4.82147100	1.55819600
H	1.70890900	2.10835900	2.16359300
H	2.75596400	3.55518700	2.06740300
H	3.10987400	2.09204400	1.07448400

Table S35. Atomic coordinates and single point energies for **46i**.



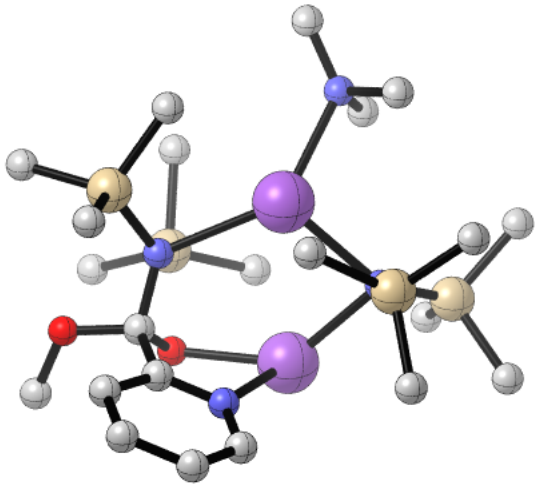
G = –2719.333755
G_{SP} = –2721.250152

N	-2.73196700	0.56054700	-0.00713500
N	2.76794900	-0.44160600	0.03779900
Na	-0.85444200	1.91812200	-0.36169700
Na	-1.04829600	-1.06546500	0.01317500
Si	-3.09708600	0.81151600	1.64340000
C	-1.93080100	-0.24376700	2.71261100
C	-4.87577400	0.41589500	2.15923600
C	-2.75368300	2.60894300	2.17539500
Si	-3.78711600	0.83172600	-1.32161800
C	-5.20334800	-0.41972700	-1.49860100
C	-2.80158800	0.76385900	-2.94596800
C	-4.60226000	2.54855300	-1.27795400
Si	3.21873700	-1.84665400	-0.94250300
C	1.64720500	-2.75348600	-1.48442600
C	4.21673800	-3.05349300	0.12179200
C	4.35500800	-1.48956700	-2.39997500
Si	2.61341000	-0.53929700	1.79523500
C	4.29821700	-0.77901400	2.60530100
C	1.47696400	-1.95916400	2.32806900
C	1.91979200	1.05567100	2.52342200
H	-1.68260500	2.86377800	2.07858500
H	-3.02101600	2.78586100	3.22888600
H	-3.33087600	3.31659500	1.55887900
H	-5.12156200	-0.63970500	1.96425200
H	-5.59640300	1.03424500	1.60078900
H	-5.03044200	0.60676100	3.23252700

H	-2.03792500	-1.32284100	2.50931600
H	-2.12134700	-0.09686400	3.78683000
H	-0.87882800	0.03587700	2.53194700
H	-5.24182200	2.72453000	-2.15696700
H	-3.84054700	3.34603800	-1.25438800
H	-5.22814900	2.66803900	-0.37886700
H	-4.83713700	-1.43117500	-1.73453000
H	-5.88801600	-0.11935300	-2.30729300
H	-5.78880500	-0.48499700	-0.56825400
H	-3.46066100	0.87449300	-3.82107300
H	-2.26341100	-0.19262200	-3.05273900
H	-2.05070500	1.57089300	-3.00638400
H	3.79843900	-1.11251200	-3.26633600
H	4.90494100	-2.39847500	-2.68884300
H	5.09422500	-0.72404700	-2.11745200
H	3.72861600	-3.38055900	1.04990300
H	5.19998600	-2.63217200	0.37997800
H	4.39707300	-3.95110600	-0.49117300
H	1.06121400	-3.00562900	-0.58426300
H	1.85890200	-3.68659800	-2.02918200
H	1.04219400	-2.09373600	-2.12377600
H	2.62917300	1.89147700	2.42554800
H	1.73427600	0.89252000	3.59711500
H	0.97558100	1.34881900	2.04509100
H	1.83650000	-2.93634300	1.97414300
H	0.45697700	-1.81579600	1.94102600
H	1.40302300	-2.00420800	3.42605200
H	4.73364700	-1.77216500	2.43839500
H	4.20065800	-0.63109500	3.69230900
H	5.00510400	-0.02517300	2.22544700
N	1.32473600	2.89391700	-0.24394400
C	1.69331000	4.16655800	-0.05208500
C	2.27233200	1.95975300	-0.36980500
C	3.01868100	4.57513800	0.01320900
C	3.63430300	2.28645600	-0.34703700
C	4.01175100	3.60657900	-0.14899300
H	0.88657700	4.89782700	0.05614900
H	3.26343700	5.62388700	0.18006200
H	5.06695400	3.88389600	-0.11686000
H	4.36080700	1.48392300	-0.47024200
O	0.55959400	0.28131800	-0.33185600
C	1.82780200	0.48636900	-0.62224700
O	2.12346400	0.28164000	-2.03078300
C	1.18396100	0.79444900	-2.92594400

H	1.55809200	0.59841000	-3.93981900
H	1.06011500	1.88899400	-2.81265800
H	0.19730100	0.31671000	-2.81008700
N	-2.08941100	-3.23004500	0.03512200
C	-3.39778700	-3.02794200	0.64530900
C	-2.21419000	-3.30640500	-1.41443600
H	-2.68298400	-2.38567000	-1.79582800
H	-1.22036300	-3.41423200	-1.87368900
H	-2.84242200	-4.16344200	-1.73244900
C	-1.43991400	-4.41747100	0.56760200
H	-0.45739100	-4.55315300	0.09425200
H	-1.29112800	-4.30859400	1.65119100
H	-2.04208800	-5.33121200	0.38583000
H	-3.30322500	-3.01476800	1.74007600
H	-4.10512400	-3.83670600	0.36904300
H	-3.81387800	-2.06240300	0.32147900

Table S36. Atomic coordinates and single point energies for **46m**.



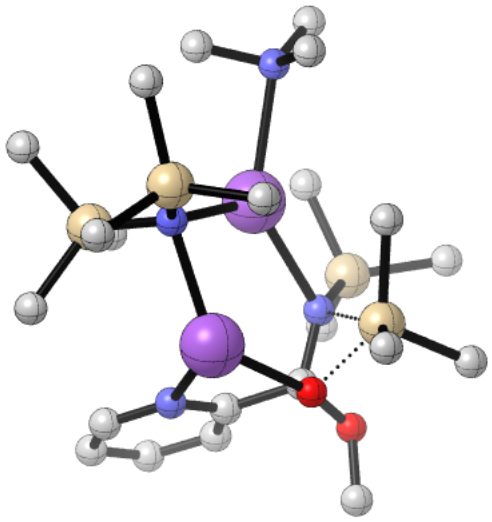
G = –2719.298927
G_{SP} = –2721.216761

N	2.21501700	0.62666300	0.23513000
N	-1.80056800	-0.64326000	0.00536000
Na	0.35809300	1.18116800	1.64148100
Na	0.65398400	-0.99921100	-0.58449000
Si	2.25533500	1.63799100	-1.15937800
C	0.75974000	1.21806300	-2.26660100
C	3.76621400	1.45258000	-2.29969300
C	2.24879300	3.50654900	-0.77845900
Si	3.63146900	0.57431600	1.22132700
C	5.07985100	-0.44696200	0.53046600
C	3.29938400	-0.13205500	2.95292900
C	4.37615900	2.29409900	1.54341700
Si	-1.46918100	-1.62182500	1.55791500
C	0.18111900	-1.48445100	2.50974800
C	-1.06507800	-3.33770900	0.72527300
C	-2.91074400	-2.13120300	2.66237100
Si	-2.59630900	-1.27375700	-1.45348000
C	-4.10013800	-2.34181200	-1.09013400
C	-1.31157000	-2.24895800	-2.44699100
C	-3.15215600	0.08312700	-2.63908800
H	1.62550400	4.07308500	-1.48739500
H	3.27365100	3.90121900	-0.85012200
H	1.89818500	3.71445300	0.24317700
H	3.90826200	0.43231500	-2.68505500
H	4.69175500	1.75124000	-1.78233800

H	3.64659000	2.12411900	-3.16557300
H	0.92710800	0.26580000	-2.80274500
H	0.62005000	1.98346600	-3.04509400
H	-0.18639600	1.14924100	-1.70323000
H	5.22089700	2.21936600	2.24616900
H	3.63686900	2.98573000	1.97824700
H	4.75545100	2.75625200	0.61864700
H	4.87525300	-1.52722500	0.50066900
H	5.96544500	-0.29810400	1.16862700
H	5.34661400	-0.12828700	-0.48867900
H	4.21944300	-0.02940200	3.54975000
H	3.02631000	-1.19764200	2.94785800
H	2.50504700	0.40817100	3.49562500
H	-3.05217300	-1.41686900	3.48445100
H	-2.74535500	-3.13535700	3.08044500
H	-3.83729700	-2.15443400	2.06887000
H	-0.16204600	-3.32551900	0.09357000
H	-1.87790300	-3.76217200	0.11607600
H	-0.86429900	-4.05361900	1.53939200
H	0.47041800	-2.46678700	2.91298100
H	0.09047600	-0.78843800	3.35907700
H	1.03508200	-1.15618100	1.89164600
H	-4.10772200	0.53479400	-2.34325300
H	-3.30274600	-0.39072600	-3.62253000
H	-2.40656400	0.88224000	-2.76132000
H	-0.83290100	-3.05957200	-1.88476800
H	-0.53152000	-1.58182800	-2.85333200
H	-1.81340000	-2.70172000	-3.31645900
H	-3.87116000	-3.20250600	-0.44712900
H	-4.54654200	-2.71626000	-2.02431000
H	-4.84066700	-1.71818800	-0.56867000
N	-1.09506400	2.56465700	0.38126000
C	-0.97894700	3.81218800	-0.08061600
C	-2.22791300	1.89322000	0.15155800
C	-1.97202500	4.45484700	-0.81259100
C	-3.28746700	2.47266700	-0.55688100
C	-3.15379900	3.76204600	-1.05656600
H	-0.04965100	4.33471600	0.14709600
H	-1.81965700	5.47499500	-1.16420700
H	-3.96909500	4.22526400	-1.61488600
H	-4.20457600	1.90444100	-0.68863500
O	-1.73849700	0.36283800	1.95258400
C	-2.36588500	0.47968700	0.76565900
O	-3.77675700	0.22054700	0.85837300

C	-4.43651500	0.85905200	1.92313800
H	-5.43914500	0.41778000	1.99444400
H	-4.53988200	1.94676600	1.75285300
H	-3.89492800	0.70357300	2.86639000
N	2.05869300	-2.93032100	-1.13096100
C	3.03868700	-2.18998700	-1.91513400
C	2.59275900	-3.24000000	0.18933700
H	2.82663700	-2.30755100	0.72415000
H	1.84956400	-3.80082900	0.77345500
H	3.52090600	-3.84452700	0.12507500
C	1.66229500	-4.14691700	-1.82284400
H	0.89012600	-4.67629500	-1.24603600
H	1.24944500	-3.89945900	-2.81069700
H	2.52350600	-4.83127400	-1.96413400
H	3.31913700	-1.27204400	-1.38039600
H	2.60784300	-1.91664800	-2.89090100
H	3.95773100	-2.78490200	-2.09607600

Table S37. Atomic coordinates and single point energies for **TS-22**.



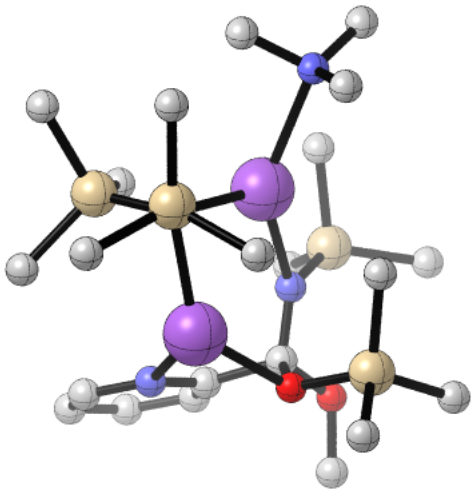
G = –2719.291865
G_{SP} = –2721.211208

N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	4.18709508
Na	1.90928846	0.00000000	1.41499763
Na	-1.27469290	-0.08203529	2.02208990
Si	-0.12870466	1.67554845	-0.37347836
C	-0.87811992	2.59342026	1.11990539
C	-1.23056015	2.16849545	-1.83974159
C	1.54908107	2.44904589	-0.85174097
Si	0.17577438	-1.12468074	-1.29877855
C	-1.34016048	-1.33204223	-2.43176042
C	0.62827371	-2.86962828	-0.71451054
C	1.57806335	-0.64511142	-2.49398934
Si	0.92279208	-1.92524074	3.79544402
C	2.10942020	-3.01232834	2.73424492
C	-0.70666342	-2.52223172	2.98295926
C	1.12173492	-2.65513142	5.51900916
Si	-1.30019641	0.36673151	5.29729481
C	-1.77116694	-1.05833529	6.44455725
C	-2.83794212	0.70223103	4.23715488
C	-1.08139967	1.88422305	6.39524087
H	1.54323713	3.54609127	-0.75353578
H	1.75212716	2.21409055	-1.90734475
H	2.40161607	2.05826463	-0.27332938
H	-2.27134910	1.82728550	-1.73645409
H	-0.83652005	1.77297820	-2.78872887

H	-1.24553799	3.26738083	-1.92239538
H	-1.96465469	2.39998492	1.16626155
H	-0.76043437	3.68328018	1.01694537
H	-0.42915575	2.31214874	2.08697007
H	1.77740876	-1.46281529	-3.20460640
H	2.51848124	-0.43086658	-1.95928222
H	1.32192007	0.24911223	-3.08413341
H	-2.18233646	-1.85195969	-1.95295586
H	-1.04295856	-1.93137167	-3.30740161
H	-1.71149529	-0.36542651	-2.80251200
H	0.52249495	-3.56536842	-1.56206739
H	0.00384767	-3.25008274	0.10786882
H	1.67776255	-2.92584085	-0.38634858
H	2.19726898	-2.72240392	5.74453758
H	0.71375247	-3.67814868	5.53776240
H	0.64722646	-2.06298097	6.30706090
H	-0.71270227	-2.30350469	1.90205149
H	-1.62490081	-2.12007791	3.44264566
H	-0.74108167	-3.62110338	3.05521228
H	1.79181912	-4.06693933	2.71802784
H	3.13462076	-2.96689574	3.13336401
H	2.15335849	-2.69776965	1.67671372
H	-0.21820503	1.75908998	7.06463852
H	-1.98460582	1.98957479	7.01698311
H	-0.95922048	2.81177025	5.81751816
H	-3.12386698	-0.17964927	3.64503638
H	-2.68013182	1.55387629	3.55253376
H	-3.70223515	0.94990975	4.87203963
H	-1.80666904	-2.02493851	5.91976843
H	-2.76542033	-0.86600604	6.87796497
H	-1.05563966	-1.15242843	7.27457548
N	2.07546378	2.04766377	2.64653194
C	2.37852826	3.29216428	2.26065521
C	1.71172669	1.84243180	3.91591472
C	2.32427144	4.39398312	3.10580660
C	1.65275725	2.89183909	4.84244093
C	1.94988631	4.18371157	4.43059581
H	2.68295811	3.42224483	1.22171172
H	2.58218898	5.38416747	2.73110904
H	1.90467253	5.01361702	5.13790131
H	1.39024031	2.66855812	5.87328094
O	2.04619459	-0.53503867	3.61176771
C	1.34766253	0.41172788	4.36335360
O	1.69734411	0.30492080	5.74213737

C	3.07340754	0.25620163	6.02585973
H	3.17331261	0.13437364	7.11174584
H	3.59075628	1.18541976	5.72493235
H	3.55555279	-0.59066737	5.51535351
N	-3.50852766	-0.99867095	1.18748798
C	-3.63275492	-0.03975264	0.09849521
C	-3.16904714	-2.31450375	0.66595050
H	-2.19897301	-2.27499859	0.15196824
H	-3.09357698	-3.03751997	1.48927753
H	-3.93116997	-2.67593309	-0.05597878
C	-4.74619691	-1.06765594	1.94798649
H	-4.62966834	-1.75837862	2.79566095
H	-5.00285321	-0.07574523	2.34436241
H	-5.58925387	-1.42438401	1.32136920
H	-2.68386590	0.01516734	-0.45277966
H	-3.86940607	0.95695722	0.50171997
H	-4.43628277	-0.32360929	-0.61309475

Table S38. Atomic coordinates and single point energies for **46n**.



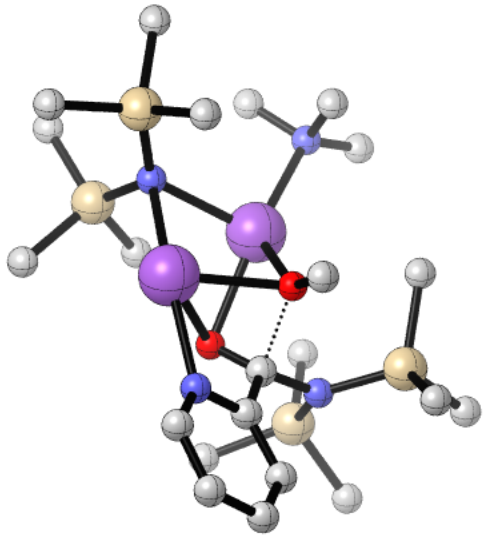
G = –2719.309158
G_{SP} = –2721.230323

N	2.20839300	0.62972300	0.16392700
N	-1.60518900	-0.54374400	-0.47834500
Na	0.26987700	1.29532000	1.26790800
Na	0.68514200	-0.94764100	-0.83557300
Si	2.28762100	1.79487300	-1.10246500
C	0.94695100	1.41167800	-2.39413900
C	3.92724400	1.88742000	-2.05224500
C	2.00713200	3.57810600	-0.48391700
Si	3.50387800	0.50120100	1.28802800
C	5.08672600	-0.32128400	0.63299800
C	3.00340000	-0.48653500	2.83378000
C	4.07720000	2.18936200	1.95261700
Si	-1.39756000	-1.24298200	2.54887200
C	-0.91790300	-0.63323500	4.25980600
C	0.03572900	-2.19804800	1.79176400
C	-2.89684400	-2.35161300	2.65696200
Si	-2.38651900	-1.48097700	-1.68806900
C	-3.32136500	-3.00960100	-1.07139800
C	-0.98535500	-2.15528300	-2.77894500
C	-3.58128200	-0.58520700	-2.85727100
H	1.62346100	4.23056600	-1.28420800
H	2.95531800	4.00729000	-0.12678900
H	1.29880900	3.62866000	0.35863000
H	4.20528300	0.92477700	-2.50772500
H	4.75234800	2.20027900	-1.39313700

H	3.84960400	2.63193700	-2.86059000
H	1.20878300	0.50755200	-2.97273300
H	0.86719700	2.23246900	-3.12322000
H	-0.05299600	1.26052600	-1.95052700
H	4.82042600	2.06308900	2.75551500
H	3.23808100	2.77698400	2.36050400
H	4.54617000	2.79432100	1.16035600
H	4.95602000	-1.38851100	0.40135100
H	5.88458500	-0.24260500	1.38859000
H	5.44240100	0.17725700	-0.28154800
H	3.79754800	-0.40346800	3.59215500
H	2.85308600	-1.55796000	2.63293000
H	2.07571500	-0.10723000	3.29480700
H	-3.73517900	-1.85618400	3.16639400
H	-2.63311500	-3.25328200	3.23195800
H	-3.22712200	-2.65004100	1.65372500
H	0.87640000	-1.53217200	1.53916400
H	-0.30465700	-2.71829800	0.88392700
H	0.42201100	-2.94222200	2.50664900
H	-0.63763700	-1.47377000	4.91243700
H	-1.76289700	-0.10504800	4.72624000
H	-0.06408100	0.06123000	4.23434400
H	-4.54468800	-0.38094300	-2.36590500
H	-3.78782300	-1.22430000	-3.73062200
H	-3.16512200	0.36711000	-3.22045200
H	-0.31904000	-2.81212700	-2.19873300
H	-0.38348300	-1.34977800	-3.23366400
H	-1.39130100	-2.76231600	-3.60212900
H	-2.67294200	-3.64954800	-0.45141500
H	-3.69247700	-3.61717500	-1.91220300
H	-4.18254600	-2.70138500	-0.46021300
N	-1.41302300	2.54188200	0.24033600
C	-1.45075700	3.77948400	-0.26701200
C	-2.41030700	1.69797700	-0.03647200
C	-2.47692500	4.24180200	-1.07986700
C	-3.48756300	2.08176800	-0.84910800
C	-3.51859200	3.36296300	-1.37792400
H	-0.61649500	4.43740300	-0.01360700
H	-2.45644100	5.26074800	-1.46519300
H	-4.34847000	3.67720000	-2.01341300
H	-4.27816200	1.36235200	-1.05165300
O	-1.67595900	0.22669400	1.72744900
C	-2.31009500	0.22462500	0.43211800
O	-3.63898200	-0.27050500	0.61078500

C	-4.44779600	0.35494400	1.57547700
H	-5.33154600	-0.28168300	1.71476200
H	-4.78151300	1.35688800	1.25552500
H	-3.92525600	0.46086300	2.53904000
N	2.26813600	-2.78694700	-1.44631300
C	3.22731800	-1.92729100	-2.12753900
C	2.77847000	-3.18709400	-0.14427300
H	2.93991700	-2.29776700	0.48040000
H	2.05203900	-3.83941000	0.36025500
H	3.74191800	-3.73253900	-0.22930100
C	1.96660600	-3.95705700	-2.25480500
H	1.20934500	-4.57705700	-1.75386700
H	1.56719100	-3.64866600	-3.23047300
H	2.87024100	-4.57810200	-2.42396700
H	3.42946600	-1.04063500	-1.51009600
H	2.81500000	-1.60098200	-3.09471900
H	4.18691200	-2.45158000	-2.31911400

Table S39. Atomic coordinates and single point energies for **TS-2**.



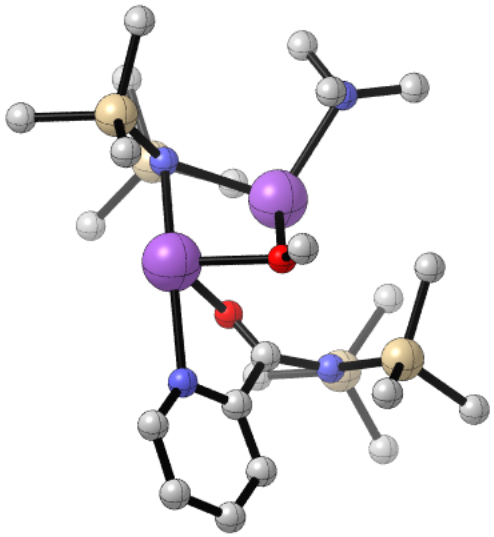
G = –2719.31406
G_{SP} = –2721.230503

N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	5.24999085
Na	1.74654089	0.00000000	1.54385881
Na	-0.94616518	-0.57626896	2.09671826
Si	-0.48835251	1.62097636	-0.27019453
C	-1.64171256	2.21026029	1.11954573
C	-1.41436382	1.91433315	-1.90203162
C	0.98526454	2.82173680	-0.24728830
Si	0.51040372	-1.04731524	-1.24846160
C	-0.86813023	-1.72681188	-2.36583442
C	1.38732021	-2.56016153	-0.49805118
C	1.79153411	-0.26683962	-2.41832478
Si	-0.37816914	-1.62689861	5.86278838
C	-1.41432459	-2.61443167	4.63583211
C	-1.48794755	-1.49776169	7.38274261
C	1.14037436	-2.55612380	6.47322418
Si	-1.01069415	1.44606556	5.60577517
C	-1.23649605	1.65401424	7.46941499
C	-2.69712106	1.25440434	4.79101496
C	-0.14388177	3.01856714	5.05433151
H	1.48966909	2.79443106	0.73413406
H	0.67464198	3.86361804	-0.42300412
H	1.72171242	2.55296424	-1.02125380
H	-2.34658941	1.32853913	-1.94098979

H	-0.80551603	1.62954354	-2.77450929
H	-1.68124282	2.97710876	-2.01262907
H	-2.53033399	1.56463616	1.21674821
H	-2.00162073	3.23338604	0.93004681
H	-1.10112931	2.21177839	2.07823033
H	2.13655068	-0.98252846	-3.18119163
H	2.67576583	0.07424083	-1.85436526
H	1.38096888	0.61045596	-2.94276977
H	-1.57812387	-2.36482326	-1.81716077
H	-0.43946933	-2.33145698	-3.18068861
H	-1.44219828	-0.90553815	-2.82230328
H	1.62490357	-3.30613546	-1.27245215
H	0.76933969	-3.05356847	0.26927822
H	2.34509181	-2.28367197	-0.02226436
H	0.86698626	-3.61069473	6.63718633
H	1.45359837	-2.14044262	7.44363033
H	1.99995982	-2.52979592	5.79496618
H	-2.46631198	-1.04013382	7.17465117
H	-1.02216641	-0.96506489	8.22244562
H	-1.67521433	-2.53417446	7.70754218
H	-2.14137992	-1.92855746	4.16969373
H	-1.98670777	-3.39771705	5.15683834
H	-0.80828831	-3.06765563	3.84356922
H	0.92051243	2.98912770	5.33681969
H	-0.60438271	3.87827903	5.56442308
H	-0.19573722	3.17031375	3.97030164
H	-3.19031440	0.32480133	5.11713093
H	-2.59761867	1.23363432	3.69448867
H	-3.35968630	2.09512770	5.04780963
H	-2.03363007	1.03942882	7.90337565
H	-1.49169954	2.70903475	7.65401562
H	-0.30176795	1.44237401	8.01174474
N	3.20868658	0.21662898	3.43115865
C	4.51903028	0.24688191	3.65061731
C	2.37658982	0.16927496	4.48018715
C	5.07998625	0.23871934	4.92892436
C	2.84431214	0.16792944	5.79386743
C	4.21983583	0.20102383	6.01990345
H	5.16330318	0.28006387	2.76734850
H	6.16217237	0.26487411	5.05382997
H	4.61156052	0.20135520	7.03832933
H	2.12793452	0.14832325	6.61348696
O	0.51957395	0.93681811	3.22015027
C	0.88645641	0.20220279	4.15887944

O	0.87203255	-1.48156521	3.16250793
C	1.71094314	-2.57963727	3.25442141
H	2.67332580	-2.34406917	3.75840314
H	1.97850268	-2.97162046	2.25377052
H	1.26457194	-3.42769542	3.81593751
N	-3.10653133	-1.55003737	1.39909120
C	-3.47055277	-0.84179814	0.17691956
C	-2.48325805	-2.82360743	1.06453406
H	-1.58070114	-2.64578501	0.46054383
H	-2.19625054	-3.35643337	1.98214165
H	-3.16433124	-3.47491598	0.47840785
C	-4.27660032	-1.74931381	2.23904263
H	-4.00419652	-2.31049491	3.14360185
H	-4.69065648	-0.77701711	2.54174052
H	-5.06885453	-2.31681051	1.70837809
H	-3.97897407	0.10000340	0.42580125
H	-4.15524274	-1.44938619	-0.45062189
H	-2.56340351	-0.61220980	-0.40012954

Table S40. Atomic coordinates and single point energies for **47**.



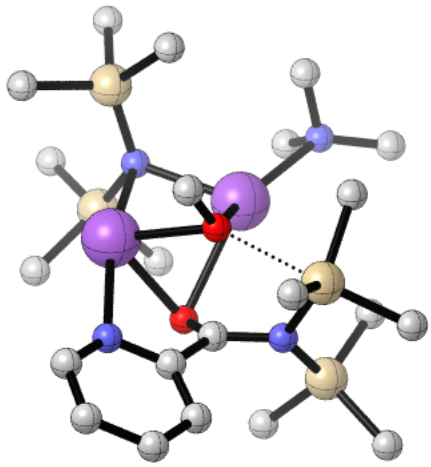
G = –2719.323886
G_{SP} = –2721.242376

N	-2.63315600	0.42584800	0.43351800
N	2.58055200	-0.45623900	0.40202700
Na	-0.82130800	1.83856000	-0.10273000
Na	-0.84039400	-0.88096400	-0.41751100
Si	-2.80487200	-0.34803300	1.94600300
C	-1.62053200	-1.84629700	2.05121500
C	-4.53256000	-1.06154300	2.28653800
C	-2.34606800	0.76113600	3.41196400
Si	-3.85794700	1.34301800	-0.31847800
C	-5.19971000	0.34063400	-1.21341100
C	-3.06972100	2.47516600	-1.64133600
C	-4.77380600	2.52981100	0.84959500
Si	3.12422000	-0.90672000	-1.25995700
C	1.85079700	-2.03894300	-2.04455100
C	4.72434700	-1.88869800	-1.10128100
C	3.50122400	0.57400600	-2.34344000
Si	2.75514300	-1.58574700	1.80234900
C	4.58739800	-1.78702900	2.19010000
C	2.00379100	-3.26343600	1.41762300
C	1.99946800	-0.80918500	3.33215400
H	-1.31342900	1.12627800	3.28973100
H	-2.41374100	0.23446200	4.37691800
H	-3.01182200	1.63752600	3.45460400
H	-4.80022300	-1.81985100	1.53335300

H	-5.30810800	-0.28022400	2.26032900
H	-4.57513300	-1.54118200	3.27715600
H	-1.82158900	-2.59214400	1.26288800
H	-1.72849800	-2.36242100	3.01764100
H	-0.57171700	-1.51753300	1.97745700
H	-5.50849800	3.14632500	0.30769500
H	-4.05880500	3.20871500	1.34196400
H	-5.31207200	1.98855800	1.64330300
H	-4.78973600	-0.24608800	-2.05019500
H	-5.97854000	1.00527400	-1.61944600
H	-5.68523000	-0.36173600	-0.51723800
H	-3.84212000	2.90926700	-2.29433400
H	-2.36125200	1.92800400	-2.28579100
H	-2.53871800	3.33543300	-1.19280600
H	3.61155200	0.20543400	-3.37597000
H	4.44462200	1.05954200	-2.05514600
H	2.69169300	1.31411000	-2.33462900
H	4.58813900	-2.86701600	-0.61804100
H	5.50908900	-1.33784100	-0.56238000
H	5.08882500	-2.07840000	-2.12354500
H	1.58514900	-2.86564700	-1.36854400
H	2.24570000	-2.47471000	-2.97559800
H	0.95340700	-1.44596100	-2.26945500
H	2.39866300	0.20612200	3.48313900
H	2.29288500	-1.41618600	4.20257000
H	0.90595800	-0.73747300	3.30147300
H	2.53480700	-3.76715100	0.59604400
H	0.93963400	-3.18204200	1.14859300
H	2.07495800	-3.90879500	2.30679600
H	5.12715100	-2.43891600	1.49321700
H	4.67842300	-2.22363800	3.19699200
H	5.09015700	-0.80766200	2.20846800
N	1.31037400	2.94596000	0.05726200
C	1.72413400	4.18606400	-0.17537500
C	2.22620600	1.99435000	0.26599500
C	3.07230800	4.55389500	-0.17931500
C	3.59377800	2.26805400	0.30622300
C	4.02303700	3.57456200	0.08038600
H	0.94893200	4.93469100	-0.36132100
H	3.35649600	5.58820000	-0.37200500
H	5.08548100	3.82104600	0.10702000
H	4.29622500	1.46073200	0.51273000
O	0.62402500	0.49356600	1.13363200
C	1.71217500	0.60425100	0.59083100

O	0.22694300	0.59687600	-1.62811600
C	0.26717200	0.97121700	-2.94210100
H	0.72104500	1.97980500	-3.10614100
H	-0.73306300	1.02441000	-3.43583600
H	0.86704700	0.27855700	-3.58744200
N	-1.94642300	-2.55089000	-1.78045800
C	-3.23166700	-2.79311200	-1.13905800
C	-2.09204100	-1.57554400	-2.85354000
H	-2.46034100	-0.62198000	-2.44351900
H	-1.11778100	-1.38622600	-3.32590500
H	-2.80476000	-1.92313500	-3.63012100
C	-1.36937600	-3.78785000	-2.27657400
H	-0.40248400	-3.58411200	-2.75671700
H	-1.20441700	-4.48583400	-1.44279800
H	-2.03073500	-4.28275200	-3.01805800
H	-3.12130500	-3.54962100	-0.34876300
H	-3.98650400	-3.15974400	-1.86577000
H	-3.59762300	-1.86062300	-0.68517700

Table S41. Atomic coordinates and single point energies for **TS-3**.



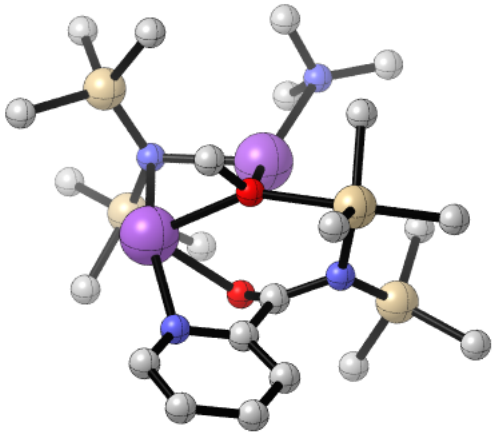
G = –2719.312343
G_{SP} = –2721.230445

N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	4.95295113
Na	1.83340062	0.00000000	1.49532365
Na	-0.91899147	-0.64216855	2.03971965
Si	0.01632305	1.68473289	-0.31785453
C	-1.25150553	2.63361455	0.72884022
C	-0.31090467	2.18659739	-2.11692352
C	1.71913762	2.44444756	0.11542013
Si	0.31494273	-1.22121011	-1.15410414
C	-0.81308782	-1.21659530	-2.68035607
C	0.13140441	-2.97115190	-0.39772671
C	2.10039388	-1.13315291	-1.81823216
Si	-0.01691598	-1.81455709	5.15185335
C	-1.23604583	-2.78930618	4.06502749
C	-0.95602154	-1.97605537	6.81752943
C	1.61039165	-2.62717845	5.65719646
Si	-1.27926577	1.12769579	5.51714297
C	-1.40649068	1.15892051	7.39470718
C	-2.92153674	0.64578186	4.74493562
C	-0.81397419	2.87604636	5.01295383
H	1.90148077	2.46091895	1.20327858
H	1.77831951	3.48883004	-0.22808219
H	2.53972913	1.89824071	-0.38290052
H	-1.29510255	1.82747187	-2.45586331
H	0.45014091	1.78044040	-2.80199425
H	-0.29911303	3.28384475	-2.21320760

H	-2.25772423	2.58652515	0.28617236
H	-0.97156562	3.69639637	0.80359373
H	-1.29524396	2.23222598	1.75381609
H	2.30303698	-1.92356354	-2.55814304
H	2.84020115	-1.25484464	-1.00649454
H	2.29434099	-0.16152940	-2.30077036
H	-1.87533267	-1.22118557	-2.38541748
H	-0.63080492	-2.11443940	-3.29239309
H	-0.64790056	-0.33469961	-3.31547211
H	1.05570873	-3.55507445	-0.53093904
H	-0.67765423	-3.53475694	-0.88841154
H	-0.08390244	-2.94751613	0.68259642
H	1.47831695	-3.72000566	5.59791921
H	1.82171675	-2.38309978	6.70915729
H	2.48221656	-2.35930951	5.05158040
H	-2.01520317	-1.67476639	6.77367085
H	-0.47675229	-1.43214023	7.64553938
H	-0.94534139	-3.04733340	7.08036410
H	-1.98977054	-2.09776572	3.64878014
H	-1.79407477	-3.51791200	4.67256553
H	-0.74528375	-3.30780470	3.23077417
H	0.20600086	3.12411717	5.34696830
H	-1.50589811	3.57657335	5.50518986
H	-0.85780840	3.03400717	3.92832321
H	-3.19681012	-0.39103696	4.99071049
H	-2.86065336	0.73439666	3.64735199
H	-3.73216291	1.30560830	5.09039415
H	-1.95500610	0.31101149	7.82055508
H	-1.92929839	2.08458140	7.68182100
H	-0.40662136	1.18690234	7.85462313
N	3.24751419	0.38732487	3.39667384
C	4.54796070	0.33013901	3.66710403
C	2.38324789	0.40721876	4.41726305
C	5.05582735	0.31065363	4.96775029
C	2.79246265	0.38629190	5.75032909
C	4.15705613	0.34314802	6.02834072
H	5.22579685	0.29960135	2.80953952
H	6.13206971	0.26915368	5.13365512
H	4.51183531	0.33066252	7.05994618
H	2.04093621	0.39696835	6.53996855
O	0.60090725	1.20331281	3.08925154
C	0.91432878	0.53615974	4.06601385
O	0.94724584	-1.54363430	3.01440347
C	1.83279267	-2.52102303	2.61395309

H	2.85613222	-2.37759054	3.02929632
H	1.95677566	-2.56447269	1.50836035
H	1.52215063	-3.54768582	2.91120674
N	-3.34144251	-1.10322483	1.49769444
C	-3.66579550	0.03783025	0.65073476
C	-3.04570239	-2.26510972	0.67100286
H	-2.24908717	-2.01651162	-0.04168475
H	-2.70878477	-3.10349481	1.29927399
H	-3.93556199	-2.59336346	0.09484554
C	-4.44318742	-1.40415449	2.39789687
H	-4.16953122	-2.23217285	3.06833251
H	-4.68775461	-0.52584841	3.00908744
H	-5.35228319	-1.70123878	1.83535246
H	-3.86055324	0.92410763	1.27219671
H	-4.56403766	-0.15800380	0.02923037
H	-2.81360700	0.25404678	-0.01070058

Table S42. Atomic coordinates and single point energies for **48**.



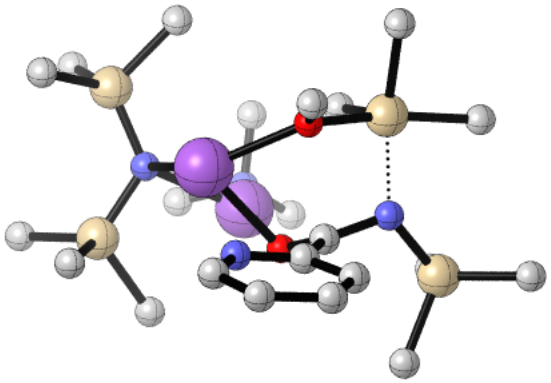
G = –2719.312695
G_{SP} = –2721.231277

N	2.44842800	0.59637400	-0.16532600
N	-2.25723100	-0.61361800	-0.28879600
Na	0.55237300	1.99259600	-0.01029200
Na	0.73540800	-0.92183000	0.24937800
Si	2.75696500	0.90698600	-1.82589500
C	2.05183400	-0.43885200	-2.96322800
C	4.58116900	1.08900600	-2.30879000
C	1.93042600	2.54266600	-2.37877500
Si	3.51148300	1.00037800	1.11322100
C	5.27192300	0.30414800	0.97368800
C	2.86344500	0.37533900	2.80440300
C	3.70866000	2.88684800	1.30504700
Si	-2.31982200	-0.82020300	1.55316000
C	-1.00690600	-1.93401900	2.39898900
C	-3.70719000	-2.17676200	1.57814800
C	-3.29837900	0.46782600	2.55155700
Si	-2.54008600	-1.87427200	-1.53006900
C	-4.32690200	-2.46198000	-1.56998700
C	-1.37097600	-3.31593700	-1.24156000
C	-2.21779600	-1.12767500	-3.22510500
H	0.83109900	2.46278500	-2.41987400
H	2.26145900	2.81888700	-3.39180300
H	2.21127600	3.37892500	-1.71400000
H	5.15213900	0.18011600	-2.06369000
H	5.06122900	1.93792800	-1.79673400
H	4.66570300	1.25950400	-3.39378200
H	2.72834600	-1.30346700	-3.03442700

H	1.91168100	-0.04352900	-3.98180900
H	1.06750900	-0.78403700	-2.60937800
H	4.38606200	3.14776100	2.13347600
H	2.74012300	3.37586300	1.51439200
H	4.11436400	3.33542300	0.38378300
H	5.25738400	-0.78393400	0.79703100
H	5.82387900	0.48420400	1.91010200
H	5.83902000	0.76658100	0.15374300
H	2.71490700	1.21269400	3.50428800
H	3.58539500	-0.31115200	3.27385100
H	1.90245100	-0.15724000	2.72664200
H	-3.19037100	0.23314000	3.62365400
H	-4.36734100	0.37143600	2.31086800
H	-3.00222900	1.51356300	2.40568800
H	-3.41001500	-3.15241100	1.15736100
H	-4.63928400	-1.86083500	1.08367500
H	-3.94942000	-2.35868200	2.63939700
H	-0.49971300	-2.53005500	1.61750700
H	-1.47970100	-2.66577000	3.07042500
H	-0.23711200	-1.38066500	2.95594500
H	-2.81511400	-0.21416400	-3.37450800
H	-2.52476600	-1.85546500	-3.99186700
H	-1.16409800	-0.86627400	-3.38375700
H	-1.48656700	-3.73647000	-0.23144300
H	-0.32607500	-2.98300800	-1.36005500
H	-1.54762300	-4.12234200	-1.96989800
H	-4.57753500	-3.17459500	-0.77592600
H	-4.50037000	-2.95066900	-2.54149900
H	-5.02142500	-1.61090000	-1.49769900
N	-1.64446400	2.93294100	-0.22226200
C	-2.24423000	4.09267900	0.03186000
C	-2.40566800	1.84811900	-0.40328900
C	-3.63169400	4.23399800	0.09675300
C	-3.79824100	1.88485400	-0.34497400
C	-4.42179700	3.10605000	-0.09912100
H	-1.59319100	4.95659600	0.19169200
H	-4.07224100	5.20951200	0.30132700
H	-5.50970900	3.17323500	-0.05331400
H	-4.36234600	0.96180000	-0.48095300
O	-0.67941500	0.61111700	-1.43251700
C	-1.68521900	0.55504300	-0.73675300
O	-0.72103500	0.51157000	1.39348300
C	-0.43929400	1.32119800	2.48333200
H	-1.06731100	2.23585400	2.50735200

H	0.61783800	1.65695800	2.48494000
H	-0.58920900	0.80816900	3.45599200
N	1.92037900	-3.14929900	0.42624500
C	2.80346800	-3.09195100	-0.73172000
C	2.66857900	-2.82844600	1.63380100
H	3.15476100	-1.85164200	1.51773600
H	1.99184000	-2.78600200	2.50027300
H	3.45466300	-3.58464400	1.83848700
C	1.32590300	-4.47098800	0.55271800
H	0.61798400	-4.48852000	1.39445500
H	0.78460600	-4.73627400	-0.36437300
H	2.10086200	-5.24356600	0.73614000
H	2.23632000	-3.30880900	-1.64875600
H	3.63121200	-3.82656300	-0.65051400
H	3.23060800	-2.08140200	-0.81464200

Table S43. Atomic coordinates and single point energies for **TS-4**.



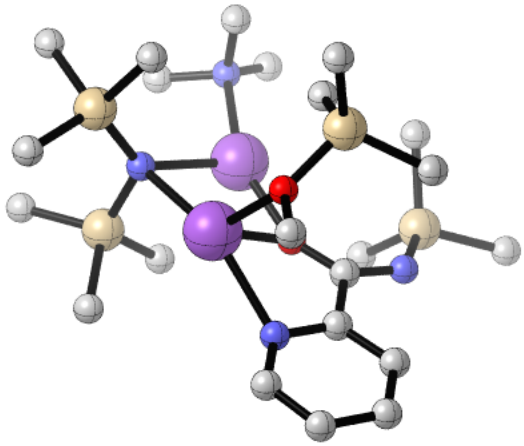
G = –2719.299499
G_{SP} = –2721.218382

N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	5.22433636
Na	1.50749994	0.00000000	1.79329724
Na	-1.57410094	0.22976535	1.68149310
Si	0.05076149	1.61185494	-0.58504426
C	-1.14617865	2.70474325	0.41822436
C	-0.40920513	1.83429359	-2.41027552
C	1.76068122	2.40689292	-0.34002316
Si	0.46103724	-1.35794075	-0.93891857
C	-0.72483086	-1.80591070	-2.35169973
C	0.61835630	-2.91276137	0.14016778
C	2.17190795	-1.12600046	-1.74058150
Si	0.15665767	-1.91611295	4.73007930
C	-1.07412329	-2.07785097	3.28959753
C	-0.94724324	-2.35956882	6.26669193
C	1.13342742	-3.58079130	4.87587129
Si	-1.33511772	0.79909449	6.07276788
C	-1.33214502	0.44204808	7.91964698
C	-3.03374353	0.47085185	5.30786556
C	-1.06095483	2.66382498	5.90602867
H	1.99965639	2.48073285	0.73477942
H	1.80422475	3.42572255	-0.75565925
H	2.54390985	1.80803283	-0.83232487
H	-1.43023627	1.47522096	-2.61412495
H	0.27692005	1.27978058	-3.06958747
H	-0.36176978	2.89690102	-2.69545676
H	-2.19579874	2.37488362	0.33268368
H	-1.11409109	3.74277078	0.05373260

H	-0.85837062	2.72542697	1.48222855
H	2.47731558	-2.01333673	-2.31675961
H	2.94626280	-0.94641909	-0.97488638
H	2.18272105	-0.26180349	-2.42406735
H	-1.71935722	-2.09933724	-1.98101697
H	-0.32701332	-2.65188728	-2.93427207
H	-0.86102033	-0.95743792	-3.03932408
H	1.07426133	-3.72915582	-0.44169532
H	-0.35917141	-3.27109539	0.49866332
H	1.24652526	-2.75285556	1.03368639
H	1.66098207	-3.83676534	3.94507888
H	0.42748730	-4.39149750	5.10695272
H	1.87686643	-3.57170455	5.69039713
H	-1.88657444	-1.79687970	6.35651696
H	-0.38871816	-2.23085114	7.20901246
H	-1.21879824	-3.42349954	6.19912550
H	-1.95350911	-1.43676072	3.47090811
H	-1.43532101	-3.11680130	3.23037142
H	-0.61725729	-1.84734868	2.31425451
H	-0.12700660	2.98990750	6.38883574
H	-1.88990458	3.19467961	6.39941703
H	-1.03311437	2.98859672	4.85519269
H	-3.32169621	-0.58938272	5.30893971
H	-3.03917937	0.83216870	4.26594664
H	-3.80572113	1.03478174	5.85468113
H	-1.77232480	-0.52684194	8.18430375
H	-1.89976438	1.23350934	8.43333076
H	-0.30123083	0.46218477	8.30517371
N	2.54247331	1.68229113	3.26475797
C	3.74008068	2.25196321	3.36038857
C	1.87741815	1.39196986	4.38814385
C	4.33542731	2.56576237	4.58380183
C	2.40426891	1.63047050	5.65641525
C	3.65408396	2.23957293	5.75249087
H	4.25556309	2.46615781	2.41938039
H	5.31610727	3.04046216	4.61016022
H	4.09290863	2.45097731	6.72882106
H	1.83298416	1.32606912	6.53309914
O	-0.10451769	1.05351013	3.17568817
C	0.50052381	0.77435632	4.21592186
O	1.59154294	-1.25039168	3.70607256
C	2.90188835	-1.42302869	4.16182316
H	2.99849065	-1.24244236	5.25001934
H	3.57716571	-0.70335623	3.66209690

H	3.28913847	-2.43540292	3.95903738
N	-3.66709698	-0.51616104	0.76938158
C	-3.68821336	0.08212032	-0.56035885
C	-3.38835652	-1.94317364	0.66238949
H	-2.40006952	-2.09297777	0.20235022
H	-3.37898175	-2.40403332	1.65907306
H	-4.14628311	-2.46050257	0.03922677
C	-4.91803931	-0.28269991	1.47415182
H	-4.86703625	-0.71713458	2.48280609
H	-5.09929723	0.79724139	1.57068187
H	-5.78109182	-0.73399260	0.94350632
H	-3.92589454	1.15304851	-0.49060123
H	-4.44778674	-0.39877253	-1.21004397
H	-2.69849891	-0.03021541	-1.02898025

Table S44. Atomic coordinates and single point energies for **49**.



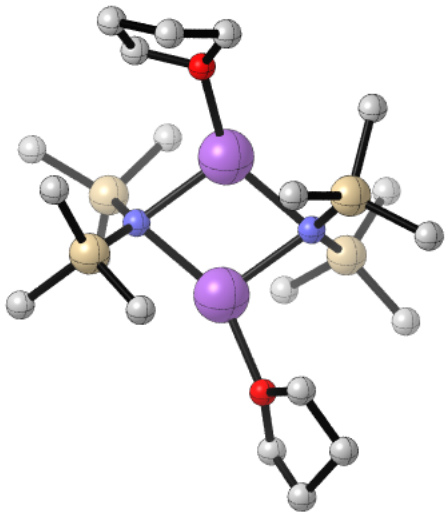
G = –2719.361990
G_{SP} = –2721.284031

N	2.22480700	0.72195300	-0.37715400
N	-2.91048800	-1.57120500	-0.55561400
Na	0.00239100	1.53153900	-0.44570400
Na	1.06724100	-1.28736000	-0.14159800
Si	2.55441100	0.60269200	-2.05807500
C	1.81945100	-1.00786200	-2.76196100
C	4.38869400	0.61512100	-2.53560700
C	1.70039800	1.98685100	-3.04757200
Si	3.16359100	1.69617500	0.67213100
C	4.87382800	0.98689900	1.09700300
C	2.30329300	1.98622300	2.34354300
C	3.45995900	3.44393600	-0.01980100
Si	-1.62229500	1.10675200	2.63822700
C	-0.44026100	-0.32007000	2.40877800
C	-3.39901800	0.53451900	2.51542900
C	-1.30554100	2.02436000	4.24217300
Si	-2.35897000	-3.20300800	-0.33796800
C	-3.88537200	-4.29939100	-0.31552000
C	-1.42037900	-3.53378000	1.28066200
C	-1.22977000	-3.75472100	-1.75005400
H	0.60129500	1.90074600	-2.98094600
H	1.95755700	1.94239000	-4.11738200
H	1.99609700	2.97930900	-2.67141700
H	4.92010100	-0.23451200	-2.07842400
H	4.89092200	1.53805800	-2.20676100
H	4.50710500	0.53861200	-3.62769100

H	2.25599600	-1.91539100	-2.30895000
H	2.01373400	-1.07389900	-3.84316400
H	0.72505800	-1.02842500	-2.62439500
H	4.05789000	4.05924600	0.67059900
H	2.49950600	3.96203800	-0.18173300
H	3.98599400	3.41838800	-0.98724900
H	4.79350200	0.04661500	1.66570600
H	5.44847000	1.69685100	1.71264200
H	5.45770800	0.77905800	0.18716400
H	2.86559200	2.73773600	2.92011000
H	2.25286800	1.07409500	2.95935400
H	1.27617600	2.36622000	2.21123000
H	-0.26175800	2.36838600	4.29142000
H	-1.48595700	1.35815700	5.09966700
H	-1.96485200	2.89719500	4.35866100
H	-3.63124800	-0.13632400	3.35752300
H	-3.55510200	-0.03138600	1.58266100
H	-4.11294800	1.37099900	2.55197800
H	-0.85999000	-0.99521200	1.65190900
H	-0.30321600	-0.87398500	3.35010400
H	0.54143200	0.04913800	2.07433300
H	-1.72106500	-3.59441400	-2.72150700
H	-0.98737100	-4.82556300	-1.66314400
H	-0.28474400	-3.18934400	-1.76744000
H	-1.95111800	-3.12293500	2.15301500
H	-0.40353700	-3.10937500	1.27677400
H	-1.32260500	-4.62197800	1.42465200
H	-4.54631900	-4.01753100	0.51812200
H	-3.62701600	-5.36356400	-0.20719200
H	-4.45574600	-4.17405700	-1.24786600
N	-2.06805600	1.75655200	-1.63588000
C	-2.65906400	2.85125100	-2.11660800
C	-2.82986400	0.71964700	-1.26614900
C	-4.03984900	2.98738000	-2.22812500
C	-4.22768600	0.76999800	-1.33350800
C	-4.83934100	1.92242200	-1.81231900
H	-1.99731800	3.66715000	-2.42507800
H	-4.47156600	3.90458600	-2.62870900
H	-5.92710200	1.98765800	-1.87457200
H	-4.78005700	-0.11483600	-1.01957400
O	-0.86186300	-0.50780900	-0.72967700
C	-2.13536700	-0.56782000	-0.80554400
O	-1.29616800	2.17558600	1.34962700
C	-2.14774800	3.28044800	1.13568600

H	-3.11939600	2.96181800	0.72022700
H	-1.67546100	3.96472600	0.41622000
H	-2.32494500	3.84162000	2.06907300
N	2.62460400	-2.88795500	0.70762100
C	3.86758000	-2.55130900	0.02303700
C	2.65075200	-2.38085200	2.07285200
H	2.79439500	-1.28869500	2.05822700
H	1.69856500	-2.60345800	2.57759100
H	3.47409100	-2.82956700	2.66560100
C	2.38270900	-4.32213000	0.68221900
H	1.43584200	-4.55423700	1.18933700
H	2.31130500	-4.67003800	-0.35792600
H	3.19604600	-4.88451100	1.18482700
H	3.85419400	-2.95498400	-0.99919400
H	4.74839800	-2.97180700	0.55028200
H	3.97408800	-1.45760800	-0.03287600

Table S45. Atomic coordinates and single point energies for **52**.



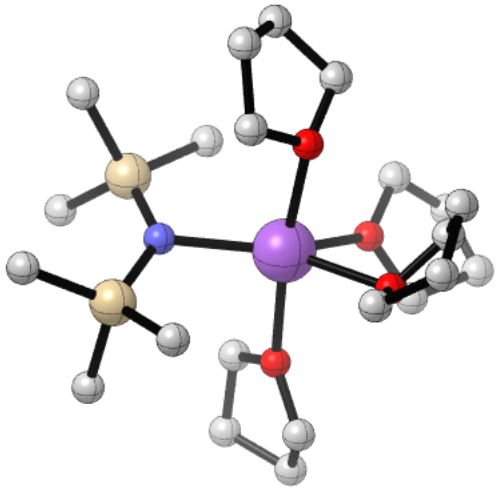
G = –2533.804958
G_{SP} = –2535.52468

N	1.26875900	1.18450700	-0.50175800
Si	1.17413400	2.58397100	0.47104200
C	0.21988700	2.16678500	2.06560300
C	0.22254400	3.99273400	-0.38997600
C	2.82179800	3.35373500	1.00633700
Si	2.31542300	0.96118000	-1.83433300
C	4.16191800	1.02056800	-1.39996000
C	2.03108300	2.18012100	-3.25665100
C	2.06022100	-0.79319300	-2.54396500
Na	-1.06091500	0.88146300	-0.69115500
Na	0.95858300	-1.07095700	0.01796200
N	-1.34893500	-1.39655000	-0.22787800
Si	-1.66059900	-2.10873400	1.29452700
C	-3.18902600	-1.40556700	2.17144900
C	-0.19065000	-1.76861700	2.46305900
C	-1.84683400	-3.99591900	1.26548800
Si	-2.06660500	-1.89061900	-1.69983600
C	-2.02462400	-0.42978300	-2.93334200
C	-3.89989200	-2.37455600	-1.58122200
C	-1.18507100	-3.34960000	-2.52406800
O	-2.84681600	2.05754400	-0.01622800
C	-3.05038100	3.17292900	0.84215300
C	-4.03162700	1.25241200	-0.02842200
C	-3.91811100	2.61555200	1.95996700
C	-4.86810100	1.69091600	1.18801700

H	-2.06790500	3.53793800	1.16697400
H	-3.56743900	3.98124600	0.29376000
H	-3.71030800	0.20156400	0.02745100
H	-4.57203500	1.40828400	-0.97619300
H	-5.20231500	0.83353000	1.78618500
H	-5.75941300	2.24508200	0.86241600
H	-4.44063500	3.39510000	2.52885200
H	-3.29010800	2.04067100	2.65749800
O	2.97219000	-1.62975300	0.85373600
C	3.34501100	-0.68002300	1.86245600
C	4.06283300	-2.49478300	0.54314100
C	4.84917800	-0.85426000	2.05217700
C	5.04349100	-2.32990400	1.69806500
H	5.17429000	-0.60082000	3.06903000
H	5.40086100	-0.21626800	1.34563400
H	4.74689700	-2.96941200	2.54293600
H	6.07381900	-2.58261900	1.41739200
H	3.67934300	-3.51839900	0.43121000
H	4.51664500	-2.18080900	-0.41299400
H	3.05325100	0.32166700	1.51223500
H	2.78834500	-0.91375500	2.78575000
H	-0.72857300	1.63523700	1.86673800
H	-0.01969200	3.06921300	2.65082700
H	0.82774100	1.50912200	2.70811900
H	-0.74631600	3.65925300	-0.79859300
H	0.81127400	4.37233200	-1.23968000
H	0.02725400	4.84061800	0.28658700
H	3.49465100	2.61731200	1.47288700
H	2.65385200	4.16632800	1.73063100
H	3.34802100	3.78401800	0.13975900
H	4.46893900	1.99873700	-1.00111500
H	4.78716100	0.79978200	-2.27965100
H	4.37658700	0.25973500	-0.63231700
H	2.28386300	3.20535900	-2.94247600
H	0.97462100	2.18110100	-3.56987500
H	2.64851500	1.93805300	-4.13564600
H	2.48091200	-1.56960800	-1.88031700
H	2.58053400	-0.89900600	-3.50794900
H	0.99820200	-1.02886000	-2.72289500
H	-2.67569000	0.39974400	-2.60283100
H	-2.40294100	-0.74426300	-3.91768700
H	-1.00881300	-0.03110800	-3.10168800
H	-0.11783400	-3.13415800	-2.68972100
H	-1.63436200	-3.60926500	-3.49525200

H	-1.24893800	-4.23627100	-1.87358900
H	-4.51930200	-1.53803700	-1.22159600
H	-4.05036700	-3.21956600	-0.89167000
H	-4.28844600	-2.67760000	-2.56629700
H	-3.07750800	-0.31801000	2.31513000
H	-3.33998800	-1.86530400	3.16047700
H	-4.09811400	-1.58058100	1.57320600
H	-2.69859300	-4.31768600	0.64673600
H	-1.99953000	-4.39850400	2.27922400
H	-0.93982000	-4.46225300	0.84883100
H	0.05790200	-0.69408300	2.49941100
H	0.71541800	-2.33008400	2.17410400
H	-0.43486300	-2.07673300	3.49110500

Table S46. Atomic coordinates and single point energies for **53**.



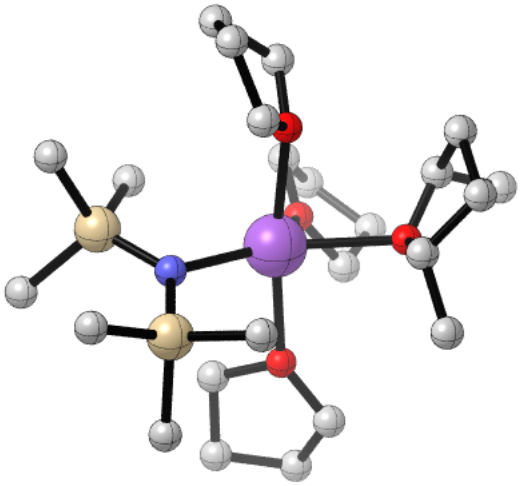
G = –1963.108437
G_{SP} = –1964.762125

N	1.94890500	0.03967200	0.03812200
Si	2.49726700	0.32520600	1.60668400
Si	2.80587600	-0.45095100	-1.33235600
C	0.98941800	0.38265000	2.77600500
C	3.43564400	1.96757600	1.83082100
C	3.65316200	-1.00808000	2.31990900
C	3.13590800	-2.32555000	-1.42094600
C	4.49249000	0.39920600	-1.55239900
C	1.79863600	-0.07890700	-2.90434700
H	2.86442900	2.81672100	1.42270900
H	4.39005000	1.92775200	1.28186200
H	3.66195300	2.18221600	2.88769100
H	0.25185400	1.11966400	2.41478100
H	1.25070800	0.64463000	3.81329700
H	0.49444400	-0.60337200	2.78396500
H	5.16376000	0.15327500	-0.71326800
H	4.37353600	1.49461300	-1.56844800
H	4.99467900	0.09482500	-2.48446000
H	0.82473600	-0.59529500	-2.85060600
H	2.30898800	-0.42340700	-3.81757700
H	1.61041600	1.00234700	-3.00894800
H	3.61218600	-2.69324700	-0.49747300
H	3.78121500	-2.59494800	-2.27212800
H	2.17680400	-2.85450400	-1.54293900
H	3.16655300	-1.99694500	2.31699200
H	3.95792200	-0.78312900	3.35454600

H	4.56806400	-1.08914300	1.71050500
Na	-0.34256500	-0.00178100	-0.12267900
O	-2.17350200	0.30553600	-1.60304500
O	-0.35113900	-2.25451300	-0.52779400
O	-2.05773700	-0.63598400	1.35037500
O	-0.57372800	2.34077800	-0.07653300
C	-1.76214500	0.82152900	-2.86924500
C	-3.18951400	1.13101600	-1.03806800
C	-2.82641600	1.83924700	-3.26291800
C	-3.22448900	2.39198000	-1.89449000
H	-2.94257400	1.32313400	0.01624400
H	-4.15453500	0.59354000	-1.08027500
H	-2.45806200	3.09582200	-1.53811700
H	-4.20320200	2.88876300	-1.88320300
H	-1.66211100	-0.01375600	-3.57656200
H	-0.77499400	1.30143000	-2.76193800
H	-2.44590600	2.60229300	-3.95392600
H	-3.68271700	1.33759200	-3.73895700
C	-0.81369000	-3.17749400	-1.49976500
C	0.30529900	-2.92560600	0.55105500
C	-0.82026300	-4.53273600	-0.79799200
C	0.38335300	-4.39480200	0.13761100
H	-0.30303300	-2.78803100	1.46403500
H	1.28306100	-2.44632600	0.70553000
H	0.34943300	-5.07610100	0.99748700
H	1.31654600	-4.58416800	-0.41276900
H	-1.74779000	-4.65802800	-0.21744700
H	-0.73964800	-5.37446800	-1.49805000
H	-1.80544100	-2.85173700	-1.84911700
H	-0.12578500	-3.18250500	-2.36415000
C	-1.08075400	3.08613900	1.01910300
C	0.54577600	3.02328700	-0.66891100
C	0.73289200	4.30926600	0.14182100
C	0.08115700	3.95467500	1.47946300
H	-1.43468100	2.38099800	1.78576300
H	-1.93910800	3.70576300	0.69250600
H	0.76957600	3.35540800	2.09441400
H	-0.23954700	4.82967300	2.05945000
H	1.79044700	4.58809800	0.23631400
H	0.19922700	5.15020900	-0.32649800
H	1.40955700	2.34216400	-0.60438000
H	0.31864800	3.22599700	-1.72837900
C	-2.92811700	-1.63600300	0.81414700
C	-2.57791700	-0.13047000	2.57791600

C	-3.68856700	-1.09419600	2.98051200
C	-4.22165300	-1.51465500	1.61126700
H	-4.79928300	-2.44777300	1.62616700
H	-4.85889200	-0.72009100	1.19236000
H	-3.26804400	-1.96300600	3.50906800
H	-4.44125700	-0.62732600	3.62850500
H	-1.75956800	-0.05522000	3.30668600
H	-2.99049300	0.88157500	2.40954400
H	-3.03502200	-1.46048000	-0.26486100
H	-2.46763600	-2.62816400	0.95875800

Table S47. Atomic coordinates and single point energies for **53a**.



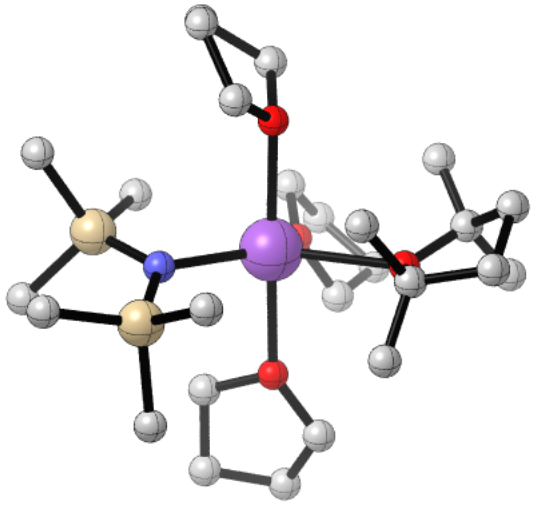
G = –2041.594084
G_{SP} = –2043.334788

N	2.09724700	-0.09198700	0.03624500
Si	2.72716700	-0.36797900	-1.50673200
Si	2.95000400	0.32367600	1.43763200
C	1.29290100	-0.39285100	-2.76516500
C	3.64812100	-2.02331000	-1.70235600
C	3.93495600	0.95760400	-2.14735700
C	3.13940000	2.20448100	1.68195900
C	4.69975400	-0.41359500	1.55540900
C	2.03059200	-0.25919000	2.99794400
H	3.03991400	-2.86445400	-1.33266600
H	4.57531900	-2.00844000	-1.10787500
H	3.92086600	-2.23048900	-2.74973800
H	0.52654600	-1.12014400	-2.45053900
H	1.61997800	-0.65986100	-3.78234600
H	0.81110400	0.59864600	-2.80861100
H	5.33019300	-0.08443500	0.71361300
H	4.65669800	-1.51425000	1.52564900
H	5.20517800	-0.11801000	2.48856900
H	1.04672000	0.23274800	3.05300600
H	2.58061200	-0.00808500	3.91851600
H	1.86743300	-1.34936500	2.98381000
H	3.64593900	2.67057100	0.82060200
H	3.70963900	2.45371200	2.59084400
H	2.13711600	2.65536300	1.77274600
H	3.45368800	1.94865900	-2.17903400
H	4.29803200	0.72675600	-3.16173300

H	4.81315900	1.03893000	-1.48702800
Na	-0.21644800	0.03976200	-0.04069700
O	-2.19158000	-0.23252800	1.31327600
O	-0.18725200	2.30960400	0.37776200
O	-1.79276700	0.64582700	-1.65635300
O	-0.45482900	-2.28224400	-0.20722500
C	-1.67264200	-0.70956300	2.56311400
C	-3.17352300	-1.12594100	0.78088100
C	-2.58182900	-1.87129300	2.96176700
C	-3.03341500	-2.41053200	1.60569700
H	-2.91871600	-1.28951400	-0.27941000
H	-2.24728100	-3.04347000	1.17370600
H	-3.96977300	-2.98318500	1.64952600
H	-0.65000700	-1.09119500	2.38267600
H	-2.05638600	-2.61448500	3.57596100
H	-3.43823500	-1.49609300	3.54440700
C	-0.75773200	3.30267100	1.21588400
C	0.64518200	2.90367200	-0.62451800
C	-0.57445500	4.62154200	0.47028800
C	0.75572000	4.37766400	-0.24507600
H	0.15464600	2.77260400	-1.60729500
H	1.60105200	2.36216300	-0.63342400
H	0.91215400	5.02670900	-1.11617600
H	1.59503900	4.52470800	0.45068500
H	-1.38506200	4.76493300	-0.26143600
H	-0.56310300	5.48968700	1.14201400
H	-1.80932200	3.04104100	1.41041300
H	-0.22152700	3.32350100	2.18170400
C	-0.92373500	-3.04427900	-1.30632100
C	0.54446200	-3.02146900	0.51524300
C	0.77206800	-4.31567600	-0.27656300
C	0.23645200	-3.96106500	-1.66551800
H	-1.20964000	-2.35148000	-2.11050200
H	-1.81891500	-3.62859000	-1.01353800
H	0.98954600	-3.39567900	-2.23536800
H	-0.07013700	-4.83498900	-2.25472700
H	1.82836900	-4.61415400	-0.28517400
H	0.18854500	-5.14468300	0.15136100
H	1.43597700	-2.37762700	0.57098200
H	0.17549300	-3.21983100	1.53627400
C	-2.61539300	1.74290200	-1.25294500
C	-2.24534600	0.11671900	-2.90007200
C	-3.20129500	1.16132600	-3.46375600
C	-3.82594200	1.70576700	-2.17932300

H	-4.29954800	2.68896500	-2.29638400
H	-4.58255700	1.00061100	-1.80082500
H	-2.63945900	1.95328400	-3.98164700
H	-3.92819800	0.73624500	-4.16752000
H	-1.37323200	-0.08607100	-3.53660900
H	-2.77927900	-0.83445100	-2.71913700
H	-2.84662700	1.62387600	-0.18511100
H	-2.05135100	2.68202500	-1.38102700
C	-1.61617100	0.43231100	3.55514400
H	-1.18295800	0.09191300	4.50636400
H	-0.99054900	1.24840200	3.16879100
H	-2.62859800	0.82195500	3.73911000
C	-4.55960000	-0.50623800	0.89707800
H	-4.57987900	0.49329300	0.44300100
H	-5.30720300	-1.13391600	0.39056100
H	-4.85137600	-0.40278900	1.95305800

Table S48. Atomic coordinates and single point energies for **53b**.



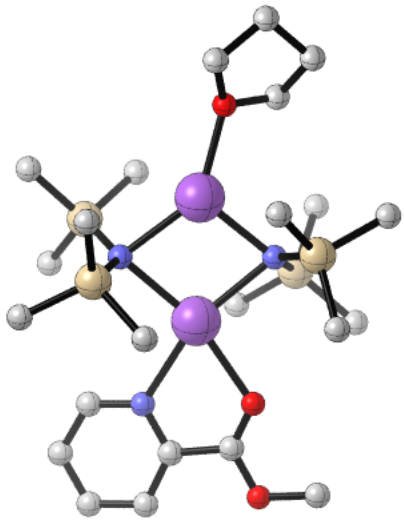
G = –2120.06819
G_{SP} = –2121.897238

N	-2.15573300	-0.06849400	0.23084300
Si	-2.91318600	0.25668400	-1.25247200
Si	-2.95960200	-0.77190000	1.55356400
C	-1.60622600	0.63148200	-2.59030200
C	-4.09405900	1.74992700	-1.23979400
C	-3.92938500	-1.16739100	-2.01602300
C	-2.68976400	-2.65808800	1.65553600
C	-4.84635500	-0.50326100	1.58950500
C	-2.40984400	-0.11488900	3.25471400
H	-3.59468200	2.65312600	-0.85550400
H	-4.95533900	1.54842600	-0.58404800
H	-4.48068600	1.97479400	-2.24690400
H	-0.88639800	1.38998900	-2.24602400
H	-2.07300500	1.00127400	-3.51736500
H	-1.03464800	-0.27832400	-2.83533200
H	-5.34361300	-0.83191800	0.66432000
H	-5.07600300	0.56561000	1.72840700
H	-5.30105200	-1.05398300	2.42851800
H	-1.40960300	-0.46480000	3.54642400
H	-3.11798500	-0.46479800	4.02290600
H	-2.40626600	0.98695400	3.27589500
H	-3.14955400	-3.16718000	0.79194600
H	-3.11864500	-3.09165000	2.57275900
H	-1.60865800	-2.88023900	1.64161500
H	-3.29411400	-2.04111500	-2.23360300

H	-4.39205800	-0.85041800	-2.96482000
H	-4.73688400	-1.50418700	-1.34831900
Na	0.17126900	0.12217900	-0.13332800
O	2.23165400	0.10738200	1.29593200
O	0.37934000	-2.24998100	-0.12605500
O	1.50572600	-0.15194500	-2.10637100
O	0.00905000	2.55501200	-0.07531100
C	1.75782500	0.15181700	2.66054600
C	3.48484200	0.80320900	1.14391900
C	3.00085100	0.54102900	3.47082600
C	3.73871300	1.46590200	2.51036600
H	3.30360200	2.47570900	2.53105600
H	4.81188400	1.55869600	2.72522800
H	2.73822500	1.01421200	4.42630800
H	3.60258100	-0.35466100	3.68876300
C	1.16347800	-3.30911200	0.40271500
C	-0.59085900	-2.75706500	-1.04991800
C	0.95046200	-4.48727900	-0.54134400
C	-0.51096400	-4.27684700	-0.94044100
H	-0.32240800	-2.40833600	-2.06448900
H	-1.56615000	-2.33262100	-0.78161500
H	-0.79310900	-4.78313300	-1.87241500
H	-1.17661700	-4.63021300	-0.13864900
H	1.60788600	-4.40283300	-1.42085300
H	1.14399600	-5.45483000	-0.06018100
H	2.20887400	-2.97166900	0.48182700
H	0.80987800	-3.56255800	1.41757900
C	0.32523700	3.41871300	-1.15510800
C	-1.07806200	3.10979700	0.68716500
C	-1.52909500	4.36983500	-0.06280400
C	-0.97577500	4.14328300	-1.47020900
H	0.70904900	2.80724000	-1.98423900
H	1.11435500	4.13602600	-0.85799300
H	-1.64205300	3.47944200	-2.04187400
H	-0.82622300	5.06994600	-2.03955400
H	-2.61916700	4.49766700	-0.04246600
H	-1.07570400	5.26954800	0.37947200
H	-1.85302900	2.33011600	0.75030300
H	-0.72642700	3.34540600	1.70296800
C	2.38721400	-1.27010900	-2.02041600
C	1.77348800	0.59807500	-3.29148300
C	2.77210800	-0.23199700	-4.09510100
C	3.52620000	-0.95898000	-2.98126100
H	4.05683000	-1.85885700	-3.31823000

H	4.25609600	-0.28246600	-2.50802500
H	2.24455300	-0.95816400	-4.73141500
H	3.41278000	0.38573200	-4.73710000
H	0.82716200	0.78695600	-3.81670700
H	2.21752000	1.56824900	-3.00649300
H	2.68138100	-1.38711200	-0.96981900
H	1.85325600	-2.18498800	-2.33037300
C	1.21026500	-1.21966700	3.01312800
H	0.84967800	-1.23196700	4.05201900
H	0.36930900	-1.47786400	2.35066500
H	1.99683200	-1.97961500	2.90133100
C	4.57989000	-0.21848700	0.84062700
H	4.35763800	-0.76644600	-0.08433100
H	5.54996900	0.28420700	0.71619400
H	4.66702000	-0.94829700	1.65885800
C	0.67816900	1.22465000	2.76587500
H	-0.18855800	0.97976300	2.13283500
H	0.31135100	1.30766200	3.79920700
H	1.07182400	2.19847000	2.44184800
C	3.33623400	1.81186500	0.01553200
H	4.26592900	2.38320800	-0.12303100
H	3.08872400	1.29168400	-0.92152600
H	2.51196200	2.50142800	0.24642000

Table S49. Atomic coordinates and single point energies for **54**.



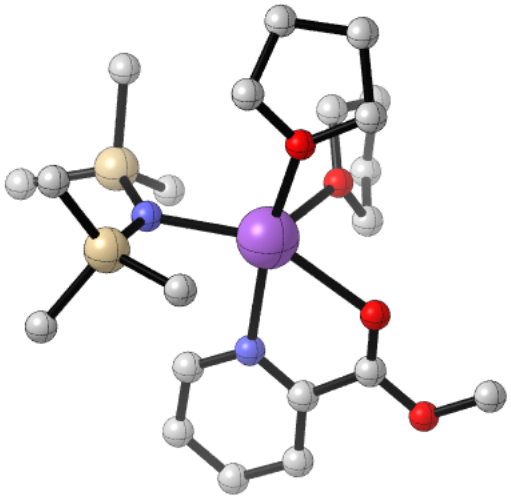
G = –2777.259118
G_{SP} = –2779.246949

Na	1.85743800	0.61162900	0.02403500
Na	-0.98998300	-0.15573400	0.00101000
N	-0.01809200	2.00314800	0.09863200
N	0.95926400	-1.49765700	-0.23040400
Si	-0.48157400	2.50625300	1.66160800
C	-1.26720200	1.03815700	2.59220100
C	-1.76798300	3.90290000	1.71673800
C	0.98428100	3.08653700	2.72111300
Si	0.39086300	3.00652700	-1.21999400
C	1.65255500	2.11146800	-2.34030000
C	1.23657500	4.63669000	-0.73595400
C	-1.07092800	3.47528900	-2.33665500
Si	1.50818600	-2.33872400	1.14704700
C	0.13723100	-3.18897200	2.14392800
C	2.34932200	-1.09777200	2.32900800
C	2.81900800	-3.67234100	0.79825800
Si	0.54612100	-2.20679900	-1.72662900
C	-0.79293000	-1.16049800	-2.60124900
C	-0.22020700	-3.93912900	-1.59474200
C	2.01133000	-2.32610500	-2.92620800
H	1.76059600	2.30523300	2.78247600
H	0.68120400	3.33744400	3.74976900
H	1.44699900	3.98115500	2.27560100
H	-2.22886500	0.74349300	2.13879700
H	-1.47205900	1.30166500	3.64109200

H	-0.60901500	0.15188600	2.60861400
H	-2.71826500	3.58702400	1.25804100
H	-1.41290600	4.79298100	1.17372800
H	-1.98292900	4.20692600	2.75332500
H	2.17261700	4.43384100	-0.19095000
H	0.59817500	5.25097400	-0.08143500
H	1.48643700	5.23982000	-1.62309600
H	-1.58509500	2.57882700	-2.71903700
H	-0.73702700	4.06823200	-3.20241800
H	-1.80250500	4.08465700	-1.78049800
H	2.65100200	2.05270500	-1.87240400
H	1.78351100	2.65440500	-3.28882500
H	1.33257700	1.08685800	-2.59579800
H	3.68899500	-3.25257500	0.26810300
H	2.40942500	-4.47712700	0.16797200
H	3.18175300	-4.13229300	1.73127000
H	1.67400600	-0.26986900	2.60703200
H	3.25251000	-0.66253200	1.86822500
H	2.66293100	-1.58318300	3.26576300
H	-0.62405000	-2.46010300	2.46371800
H	0.53590100	-3.69387900	3.03797700
H	-0.37104500	-3.93887600	1.51737200
H	2.43598800	-1.32947800	-3.12896200
H	1.72133100	-2.77341000	-3.88982800
H	2.80868600	-2.95003100	-2.49029000
H	-1.11302200	-3.88150600	-0.95215100
H	0.47332200	-4.66714600	-1.14613800
H	-0.52316800	-4.32479900	-2.58104200
H	-1.77661300	-1.28990200	-2.11776900
H	-0.91085300	-1.47754800	-3.64874100
H	-0.55709500	-0.08260700	-2.61347700
O	4.09823300	0.68505200	-0.11750300
C	5.13831800	1.22557100	0.69917000
C	4.54794900	-0.48771500	-0.80464300
C	6.37601000	0.37484200	0.41148700
C	5.75524600	-0.95957300	-0.00753800
H	5.27459300	2.28808600	0.45267000
H	4.83087400	1.14892100	1.75552100
H	4.82588400	-0.22179000	-1.83923500
H	3.71382900	-1.20593500	-0.83846600
H	6.43067400	-1.59465000	-0.59457800
H	5.42486800	-1.52745600	0.87610200
H	7.04174300	0.29728500	1.28026600
H	6.95032000	0.80275000	-0.42352400

N	-3.32889000	0.45919600	-0.30292600
C	-3.76141400	1.66781000	-0.64080600
C	-4.22394200	-0.49316800	-0.03811700
C	-5.12312900	1.97482700	-0.73355900
C	-5.60077900	-0.29151800	-0.10307100
C	-6.05425300	0.97821700	-0.46125900
H	-2.98884700	2.41421500	-0.84250300
H	-5.43499600	2.98074400	-1.01429700
H	-7.12363400	1.18412000	-0.52448800
H	-6.28253600	-1.10975400	0.12388200
O	-2.42726900	-1.98512100	0.44081100
O	-4.51620300	-2.75404500	0.58714900
C	-3.61747800	-1.81259200	0.35121000
C	-3.99613500	-4.02767300	0.96714700
H	-3.39244400	-4.44631400	0.15129800
H	-4.86376600	-4.66129200	1.17003000
H	-3.36508800	-3.92805300	1.85963400

Table S50. Atomic coordinates and single point energies for **55**.



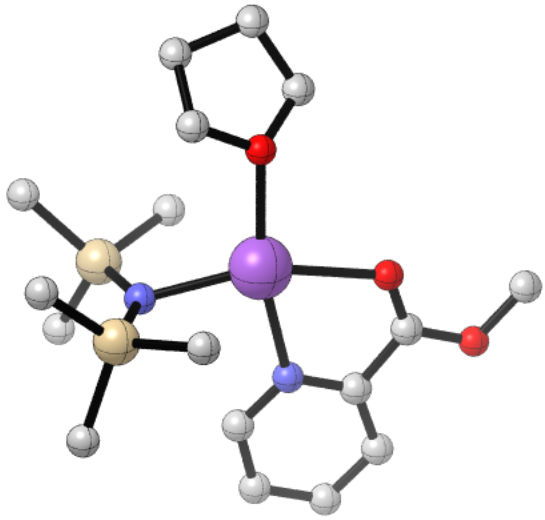
G = –1974.486739
G_{SP} = –1976.146934

N	1.52540300	-1.18038300	0.03595300
Si	1.87938800	-2.09243500	-1.34003300
Si	2.22994400	-1.08678100	1.56381700
C	0.78148100	-1.48275200	-2.77724300
C	1.51882400	-3.95476100	-1.17217200
C	3.68015800	-1.98250000	-1.94674400
C	3.58191400	0.25075300	1.69152100
C	3.04568300	-2.69004800	2.18228200
C	0.89852400	-0.64440400	2.86223400
H	0.45204600	-4.13537700	-0.96156800
H	2.10249900	-4.38655400	-0.34349300
H	1.77642200	-4.50536100	-2.09113800
H	-0.28608000	-1.60788800	-2.52293800
H	0.96338500	-2.04203600	-3.70795100
H	0.95860400	-0.41449500	-2.98891000
H	3.85785500	-3.00112600	1.50524300
H	2.31162200	-3.51137300	2.21652000
H	3.47277400	-2.57439900	3.19132300
H	0.19556500	0.08742900	2.43172700
H	1.32022600	-0.22407000	3.78978200
H	0.31288600	-1.53714900	3.13670000
H	4.40363100	0.01574600	0.99503100
H	4.00743400	0.32852600	2.70482500
H	3.18988500	1.24162200	1.40949800
H	3.96330300	-0.94296200	-2.17578900

H	3.84842700	-2.58663100	-2.85257900
H	4.36777600	-2.34762700	-1.16651700
Na	-0.14906700	0.29960200	-0.53853400
O	1.09055900	1.89731000	-1.52980400
O	-0.63368800	1.96172100	0.97121200
C	0.73165200	3.21965300	-1.88711400
C	2.49948200	1.75689400	-1.63729400
C	1.98505400	4.09153900	-1.63919100
C	3.03226600	3.08879700	-1.12141800
H	2.78362800	1.59387700	-2.69446700
H	2.78559400	0.87760100	-1.04311800
H	4.04817000	3.30776800	-1.47397000
H	3.05277800	3.07248500	-0.02200700
H	2.31890000	4.55897300	-2.57556800
H	1.79451400	4.90096200	-0.92132800
H	0.42754900	3.25217900	-2.94702200
H	-0.13546300	3.50092300	-1.27135400
C	0.37330000	2.75575900	1.59452400
C	-1.80984300	1.91166700	1.77015500
C	-1.41140100	2.49218700	3.12486400
C	-0.33662700	3.50231000	2.72070600
H	-0.80160900	4.42360900	2.33757500
H	0.34137700	3.77287100	3.53998700
H	-2.25834100	2.93850700	3.66172100
H	-0.97157100	1.70546900	3.75541500
H	-2.60140500	2.51251800	1.28810700
H	-2.15098200	0.86626600	1.83217900
N	-1.78799300	-1.35411000	0.08592500
C	-1.44396000	-2.47965200	0.70095600
C	-3.06789000	-1.14237300	-0.21465600
C	-2.39289600	-3.44772800	1.05182100
C	-4.08765200	-2.04024800	0.09351100
C	-3.73078800	-3.22154100	0.74566800
H	-0.37112100	-2.59248100	0.89299700
H	-2.07481200	-4.36183600	1.55329500
H	-4.49247500	-3.95797800	1.00603200
H	-5.11799900	-1.81447500	-0.17717300
C	-3.31465500	0.15241500	-0.93655400
O	-2.43398200	0.90842800	-1.26259300
H	1.16481700	2.09364600	1.98434700
O	-4.60099500	0.37455800	-1.17903200
C	-4.90551400	1.57555400	-1.87841100
H	-5.99317000	1.59725800	-1.99014400
H	-4.41555500	1.57835600	-2.86076500

H	-4.55783200	2.44682300	-1.30790700
H	0.81614200	3.41999600	0.83823100

Table S51. Atomic coordinates and single point energies for **55a**.

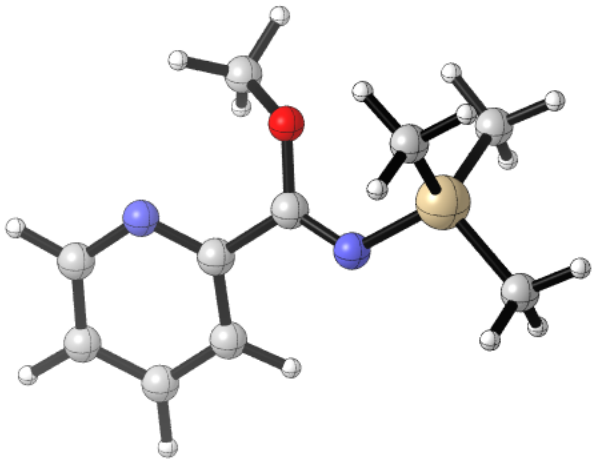


G = –1742.417049
G_{SP} = –1743.813947

N	-1.31944500	-1.00140300	0.05406400
Si	-1.73347100	-1.73082500	1.51521900
Si	-1.86197700	-0.98087500	-1.53959600
C	-0.75937500	-0.86276400	2.90965200
C	-1.28337700	-3.57588000	1.63912200
C	-3.57017300	-1.61140500	1.98900100
C	-3.72404000	-0.66130000	-1.75909000
C	-1.48879500	-2.55809500	-2.53555900
C	-0.95921300	0.43487200	-2.45365200
H	-0.19598600	-3.72833700	1.54400400
H	-1.77243000	-4.14578500	0.83290800
H	-1.59786000	-4.01185600	2.60073500
H	0.32719100	-0.94364000	2.72839500
H	-0.95654400	-1.29685200	3.90208500
H	-1.02137500	0.20858400	2.96324900
H	-1.95288700	-3.43429600	-2.05519400
H	-0.40395100	-2.74395200	-2.59203500
H	-1.87164700	-2.49480400	-3.56665500
H	-1.15739600	1.40113300	-1.95774700
H	-1.26500500	0.53170500	-3.50682700
H	0.13204200	0.26374100	-2.44198000
H	-4.30809400	-1.49930800	-1.34677000
H	-3.99984000	-0.54862300	-2.81984100
H	-4.04053300	0.24935000	-1.22528700
H	-3.91058500	-0.56351900	1.99165900

H	-3.76369400	-2.03369600	2.98796900
H	-4.19395200	-2.15873200	1.26470300
Na	0.20603400	0.66485300	0.36723100
O	-1.07675500	2.51590300	0.51052100
C	-0.88452300	3.77325600	-0.13493200
C	-2.47145300	2.24883900	0.69443900
C	-2.28096300	4.37542200	-0.30877000
C	-3.16662600	3.12803200	-0.33433400
H	-2.76486500	2.52878900	1.72172200
H	-2.62413900	1.16858200	0.55419900
H	-4.21607100	3.32932800	-0.08392500
H	-3.13278100	2.64654300	-1.32385900
H	-2.53867500	5.00265300	0.55768100
H	-2.36154400	4.99274800	-1.21263400
H	-0.21848200	4.39929300	0.47683800
H	-0.39682300	3.59820200	-1.10875900
N	1.99111500	-0.85360800	-0.10426100
C	1.77938500	-2.13786700	-0.36827500
C	3.23688300	-0.38368400	-0.10679300
C	2.83512500	-3.01439700	-0.64697900
C	4.35412400	-1.17236400	-0.37078600
C	4.13681600	-2.52334300	-0.64671900
H	0.72840500	-2.44822600	-0.35287600
H	2.62686200	-4.06304100	-0.85963800
H	4.97904800	-3.18314900	-0.86006400
H	5.35122000	-0.73460400	-0.35909000
C	3.32526100	1.08480900	0.19728200
O	2.35660000	1.77478000	0.41057800
O	4.56677500	1.54346200	0.20599400
C	4.72252200	2.93071200	0.48816900
H	5.79732000	3.12921200	0.45793300
H	4.31270300	3.16404700	1.47926300
H	4.19615300	3.53178200	-0.26444100

Table S52. Atomic coordinates and single point energies for **56**.

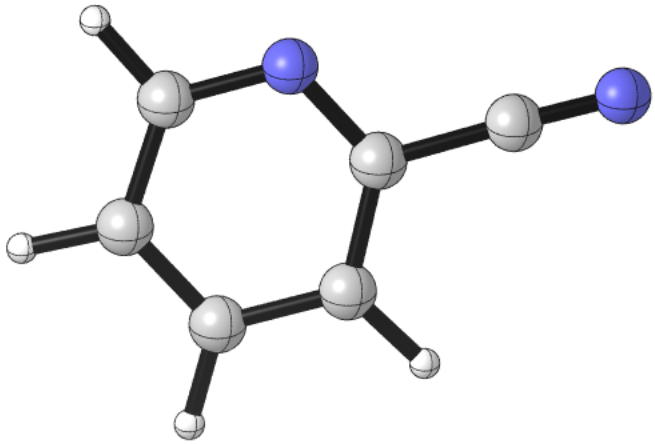


G = –863.964501
G_{SP} = –864.7163518

N	-2.45182000	0.80149200	0.45261800
C	-3.73676000	0.46222800	0.51392000
C	-1.58202900	-0.09735800	-0.00553200
C	-4.21819800	-0.78334600	0.11323600
C	-1.96063000	-1.37850300	-0.42498200
C	-3.30593000	-1.72108300	-0.36853400
H	-4.42272200	1.22082000	0.90246100
H	-5.28280100	-1.00859400	0.18016200
H	-3.64031400	-2.70839300	-0.69117900
H	-1.18886600	-2.06727500	-0.76570700
O	0.23523800	1.55866700	0.03020400
N	0.75226400	-0.66245000	0.02587900
Si	2.49647800	-0.37412700	0.06973600
C	-0.54521600	2.58939800	-0.55275500
C	-0.11556400	0.25093000	-0.00512600
H	-1.22253200	3.03331300	0.18481100
H	-1.13899800	2.21594100	-1.39864700
H	0.16649600	3.34066800	-0.91911800
C	2.94255000	0.47663700	1.68379200
C	3.02294800	0.66573100	-1.40754200
C	3.31175700	-2.06099200	-0.02162400
H	2.44336300	1.45418700	1.74389900
H	4.02931900	0.63024300	1.76451200
H	2.61818700	-0.12936900	2.54270100
H	2.58666600	1.67241900	-1.34253100
H	2.68875100	0.20285000	-2.34825200

H	4.11873300	0.76176700	-1.44771100
H	2.98757500	-2.69124100	0.81964900
H	4.40849000	-1.97810800	0.01222400
H	3.03538900	-2.57593600	-0.95381000

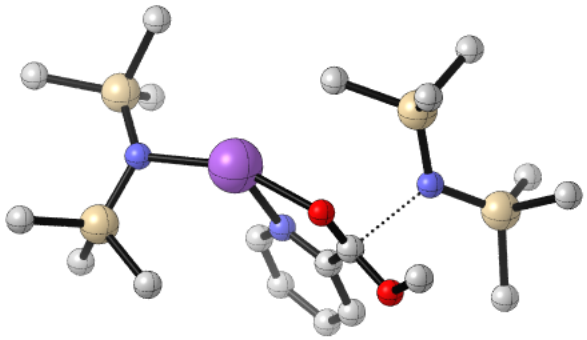
Table S53. Atomic coordinates and single point energies for **6**.



G = –340.070939
G_{SP} = –340.452349

N	0.04404400	-1.20408100	0.00000000
C	1.37134500	-1.21011800	0.00000000
C	-0.56677600	-0.01948600	0.00000000
C	2.14598200	-0.04658100	0.00000000
C	0.10617700	1.20722000	0.00000000
C	1.49782800	1.18457700	0.00000000
H	1.85118100	-2.19276300	0.00000000
H	3.23401000	-0.11308700	0.00000000
H	2.06521300	2.11610000	0.00000000
H	-0.45606900	2.14063600	0.00000000
C	-2.01976800	-0.02998800	0.00000000
N	-3.17305200	-0.00515200	0.00000000

Table S54. Atomic coordinates and single point energies for **TS-5**.

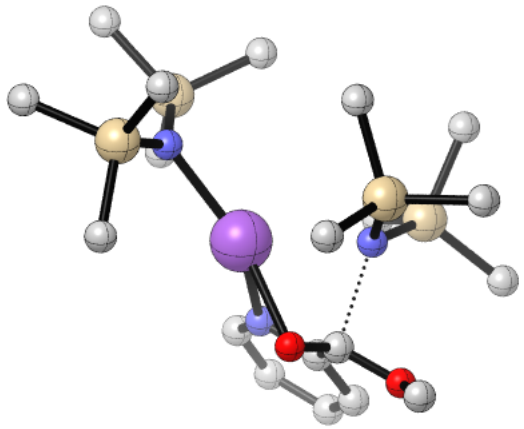


G = –2382.922559
G_{SP} = –2384.607027

Na	-1.24528800	0.49086100	0.95187300
N	-3.41479200	0.41094400	0.36614800
N	2.86682100	0.36109600	-0.05873300
Si	-4.08414500	-1.08210700	0.78166900
C	-5.62031300	-0.97994400	1.90460200
C	-2.81120100	-2.11952000	1.74896200
C	-4.62035000	-2.16611200	-0.69480300
Si	-4.03610700	1.61721400	-0.64009500
C	-3.32046600	3.31891700	-0.19128800
C	-5.93257800	1.80754600	-0.58312100
C	-3.60557500	1.35484700	-2.48003400
Si	2.47013100	1.97360800	0.28164000
C	0.62518700	2.40119200	-0.00787600
C	3.40175000	3.26269300	-0.77580000
C	2.80389100	2.47774600	2.08982400
Si	4.39203300	-0.13117000	-0.60673500
C	4.64775900	-2.01914100	-0.66362600
C	5.84104400	0.49021900	0.48052900
C	4.82437500	0.41736200	-2.38149400
H	-5.37662500	-1.64325400	-1.30331400
H	-5.05405300	-3.12514700	-0.36724000
H	-3.76068100	-2.38677700	-1.34791300
H	-2.46851600	-1.58573700	2.65201200
H	-1.92606300	-2.34286500	1.13012000
H	-3.23587300	-3.08083900	2.07931300
H	-5.38837800	-0.40422400	2.81454600
H	-5.97753200	-1.97783300	2.20759900
H	-6.44459000	-0.46388600	1.38740500
H	-2.51166300	1.37683300	-2.61727700

H	-4.04218900	2.12823800	-3.13286000
H	-3.96892700	0.37195300	-2.82331500
H	-3.57352800	3.57860300	0.84901400
H	-3.70498700	4.11575800	-0.84799600
H	-2.22129600	3.31588200	-0.27933400
H	-6.26791100	2.01979500	0.44458800
H	-6.42968500	0.87906500	-0.90973300
H	-6.28175200	2.62457700	-1.23527400
H	3.16265900	3.13298400	-1.84338400
H	4.49453600	3.17759400	-0.66479500
H	3.11042300	4.28474900	-0.48238400
H	0.15503700	1.66162700	-0.67512000
H	0.51947600	3.39041000	-0.47921300
H	0.08664600	2.45508100	0.95321600
H	2.20071100	1.84330100	2.75835500
H	2.54388400	3.53166600	2.28283700
H	3.86675800	2.33392300	2.34528900
H	4.02707100	0.09752300	-3.07137700
H	5.77397200	-0.02894900	-2.72064000
H	4.91345600	1.51130700	-2.45985600
H	4.35377400	-2.50878800	0.27693500
H	5.71440800	-2.22785000	-0.84750000
H	4.07593000	-2.47349500	-1.48751900
H	5.75574000	0.09087200	1.50476600
H	5.83800400	1.58969000	0.55571600
H	6.81997200	0.18137200	0.07793200
N	-0.28307800	-0.97059700	-0.61857500
C	-0.87635900	-1.42010400	-1.72096000
C	0.81707300	-1.57238100	-0.17444900
C	-0.39089400	-2.51412800	-2.43580900
C	1.36077200	-2.69686700	-0.79934100
C	0.74521800	-3.16485200	-1.95507400
H	-1.78656000	-0.89198100	-2.02312400
H	-0.90549200	-2.85363500	-3.33476900
H	1.14551300	-4.03745100	-2.47487700
H	2.24279600	-3.17099300	-0.37585800
O	0.74792500	-0.21266200	1.79268300
C	1.36637600	-1.02228200	1.11732700
O	2.33270200	-1.79195400	1.62296100
C	2.99470500	-1.25265800	2.74938400
H	3.78354100	-1.96437700	3.01837500
H	2.29545600	-1.11770400	3.58658200
H	3.42777500	-0.28050600	2.47002100

Table S55. Atomic coordinates and single point energies for **TS-23**.



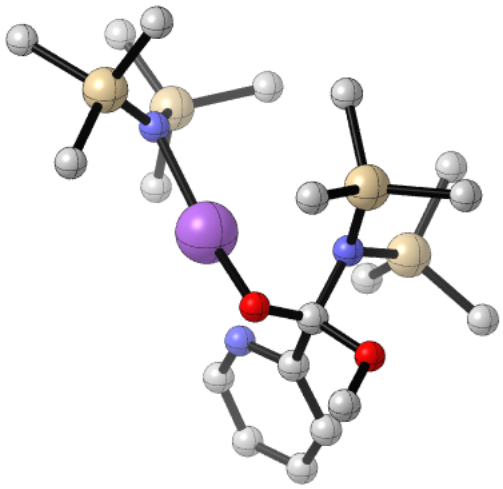
G = –2382.921687
G_{SP} = –2384.601813

Na	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.27789869
N	1.94096447	0.00000000	-1.51712643
Si	0.58670938	1.45858544	2.88402758
C	-0.29712111	2.94450264	2.07518729
C	2.42246167	1.75094139	2.47909272
C	0.41873453	1.71286249	4.76526784
Si	-0.63459594	-1.40116088	2.96549161
C	-1.91938000	-2.19683206	1.80284034
C	-1.56442197	-1.16831023	4.61603563
C	0.66726715	-2.74586102	3.32082540
Si	2.64416387	-1.45690012	-0.88859804
C	1.39694331	-2.87039905	-0.66613400
C	3.34002393	-1.25970095	0.86248909
C	4.06319684	-2.16875714	-1.95316308
Si	2.97367733	1.32822365	-1.90746130
C	2.23611789	3.03570790	-1.52132776
C	3.44723373	1.32559480	-3.74848237
C	4.63119516	1.37788211	-0.96791172
H	-0.08281488	2.94398905	0.99324819
H	0.03883001	3.91248126	2.48109506
H	-1.38868935	2.86563206	2.20449905
H	-0.63541469	1.67204581	5.08114469
H	0.83309830	2.68817863	5.06899493
H	0.96306541	0.92674849	5.31352089
H	-2.35040776	-0.40268767	4.51365898
H	-0.88358314	-0.84336361	5.41810233

H	-2.04159160	-2.10957394	4.93558001
H	1.19654730	-3.02973185	2.39757027
H	0.22231752	-3.65498921	3.75800073
H	1.42242959	-2.35807762	4.02416928
H	-2.77385113	-1.51292084	1.67228312
H	-2.30276341	-3.14847982	2.20548955
H	-1.50952730	-2.40526238	0.80049483
H	2.55295792	1.34487653	-4.38738500
H	3.99685542	0.40008145	-3.98532463
H	4.08724128	2.18519108	-4.00518778
H	4.47398271	1.59607963	0.09954755
H	5.24122012	2.19300994	-1.39093804
H	5.21340008	0.44808727	-1.04122084
H	2.52471357	-0.95530121	1.54133472
H	4.14233855	-0.51228639	0.93684159
H	3.73459669	-2.22683356	1.21708831
H	0.61996825	-2.60240085	0.06760027
H	1.94560212	-3.73143353	-0.24923257
H	0.87852256	-3.17878143	-1.58179964
H	3.75899043	-2.36951102	-2.99163433
H	4.42393910	-3.11421888	-1.51634178
H	4.91614013	-1.47435720	-1.99425672
H	1.45542910	3.35221465	-2.22725895
H	3.04196762	3.78682175	-1.55930604
H	1.80979663	3.05309250	-0.50536221
N	-0.70380934	1.70590829	-1.57800500
C	-1.21660343	2.93159294	-1.56906299
C	-0.21027227	1.21942969	-2.71746992
C	-1.27758543	3.73830400	-2.70612529
C	-0.22159310	1.95121787	-3.90850126
C	-0.76721368	3.23198373	-3.89759751
H	-1.59561801	3.29174593	-0.60831517
H	-1.71249715	4.73609474	-2.64755417
H	-0.79399938	3.82761004	-4.81223626
H	0.18157123	1.50028142	-4.81273159
O	-0.44203088	-1.04409728	-2.03936063
O	0.77040109	-0.56294996	-3.89337357
C	0.23209014	-0.23843927	-2.68143357
C	0.93318218	-1.93620592	-4.13973822
H	-0.00380314	-2.48248575	-3.95851409
H	1.71615499	-2.35779426	-3.49368737
H	1.23690323	-2.03452910	-5.18921332
H	2.74731855	2.77273287	2.73603408
H	2.58536021	1.59726648	1.39899181

H	3.06965077	1.03363491	3.00826728

Table S56. Atomic coordinates and single point energies for **60c**.



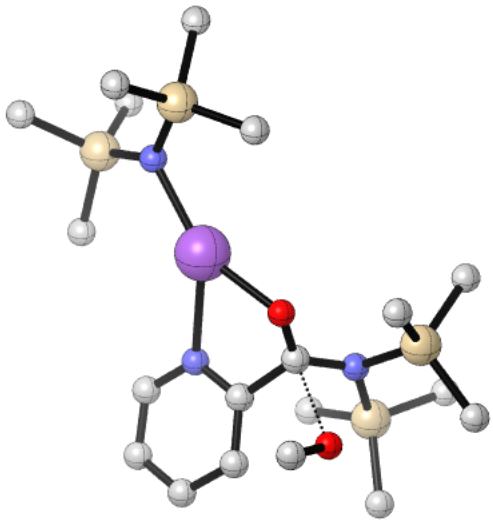
G = –2382.93489
G_{SP} = –2384.612083

Na	-0.66054600	0.39741100	-0.95394700
N	-2.79741100	0.38616300	-0.18788200
N	1.40835100	-0.73694100	0.33395400
Si	-2.90353000	1.45040200	1.11103500
C	-2.05420700	3.11031200	0.69985300
C	-1.96053300	0.81532500	2.63672400
C	-4.65942400	1.88803600	1.70375600
Si	-3.86453900	-0.57352000	-1.06895200
C	-3.25314100	-0.77269700	-2.86141400
C	-5.64203500	0.10449500	-1.21173700
C	-4.05632300	-2.34624400	-0.39724200
Si	0.79797400	-2.41222400	0.46617000
C	0.27601300	-3.22186500	-1.14744100
C	-0.73526700	-2.43502400	1.56442400
C	2.15406100	-3.55053100	1.14970600
Si	2.24083400	-0.05714400	1.73993100
C	2.02455000	1.81018300	1.95023200
C	4.09339300	-0.43177400	1.70580300
C	1.57858500	-0.76116700	3.36863700
H	-0.99748500	2.93219000	0.43404700
H	-2.07066100	3.81731200	1.54517400
H	-2.53970700	3.58816800	-0.16628800
H	-5.25266900	2.33018300	0.88804600
H	-4.63062500	2.60606900	2.53956100
H	-5.18788900	0.98471700	2.04925100

H	-5.63345600	1.12891500	-1.61764800
H	-6.13460500	0.14007000	-0.22728800
H	-6.25672000	-0.52379900	-1.87725800
H	-3.09359000	-2.88027800	-0.44064700
H	-4.79740700	-2.92933500	-0.96849800
H	-4.37261600	-2.32364600	0.65840200
H	-3.22998800	0.20682300	-3.36617800
H	-3.90098600	-1.44360000	-3.44847800
H	-2.23106700	-1.18658800	-2.89438300
H	4.56744900	0.00250300	0.81590700
H	4.25879500	-1.51836300	1.66602400
H	4.58646900	-0.02851700	2.60495900
H	0.55226300	-0.42085300	3.56850000
H	2.22486000	-0.35918800	4.16596200
H	1.60002800	-1.85626600	3.43947200
H	-1.49061800	-1.74528900	1.14766000
H	-0.55259300	-2.14273300	2.60664100
H	-1.16776900	-3.44907200	1.56279600
H	-0.56792600	-2.69576300	-1.61221100
H	-0.02500400	-4.25876500	-0.91891600
H	1.09888900	-3.22642500	-1.87307400
H	3.00350800	-3.50288600	0.45031100
H	1.79376800	-4.59060600	1.19315700
H	2.52114700	-3.27539600	2.14844900
H	2.64766700	2.40472200	1.26682000
H	2.31158900	2.06934900	2.98239600
H	0.97397600	2.10574800	1.80530700
N	1.23929500	1.96626400	-1.05098100
C	1.46593900	3.27194700	-1.13841300
C	2.27197800	1.11471200	-1.10509900
C	2.74046100	3.81568500	-1.30423800
C	3.58471600	1.56895700	-1.26935400
C	3.81857900	2.93757600	-1.37568600
H	0.58868700	3.92358000	-1.06805200
H	2.87408700	4.89531500	-1.37534600
H	4.83466400	3.31608600	-1.50772400
H	4.39346400	0.84047500	-1.30364000
O	0.98751500	-0.62404400	-1.97960700
O	3.10657900	-1.16592800	-1.22509200
C	1.87397600	-0.39153200	-1.06584500
C	3.43292800	-1.43771600	-2.55768600
H	3.67058700	-0.51788100	-3.12771700
H	2.60699100	-1.93961700	-3.08232300
H	4.32342600	-2.08412500	-2.54992900

H	-1.88518500	1.56413000	3.44220700
H	-0.93975500	0.54090900	2.32207000
H	-2.42823700	-0.09569100	3.04337200

Table S57. Atomic coordinates and single point energies for **TS-12**.



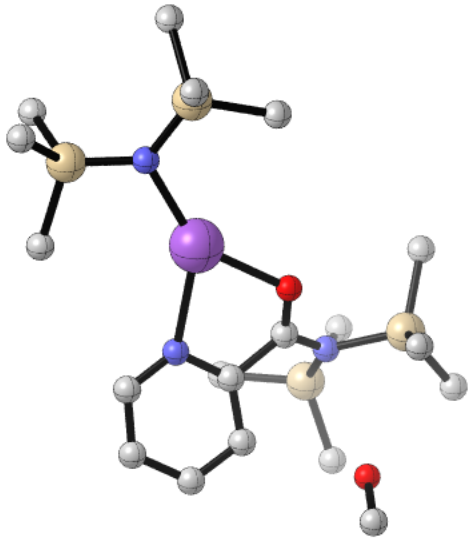
G = –2382.910172
G_{SP} = –2384.589925

Na	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.23538149
N	1.83972044	0.00000000	-3.55115132
Si	-0.47266897	1.41628291	3.02181287
C	-1.27210078	2.60719041	1.76719615
C	0.95230654	2.40152978	3.81457769
C	-1.75017304	1.17318036	4.41493181
Si	0.51800523	-1.46083515	2.91547075
C	1.33647352	-2.54402994	1.58455922
C	-0.88610347	-2.51479397	3.65445457
C	1.79448167	-1.27167743	4.31817146
Si	2.76759431	-1.53482655	-3.82580862
C	2.03138848	-3.09252611	-3.10380462
C	4.45088196	-1.30711934	-2.98579305
C	2.98136180	-1.78484076	-5.67912270
Si	2.12549447	1.39872788	-4.61695222
C	1.56135709	3.00045128	-3.78764344
C	1.32458148	1.15434420	-6.30511024
C	3.99204473	1.60483946	-4.81044174
H	-0.55330949	2.85351071	0.96675660
H	-1.59477993	3.55352532	2.22970525
H	-2.15455564	2.13545051	1.30373705
H	-2.62852572	0.62292761	4.04223372
H	-2.09276597	2.13223872	4.83649824
H	-1.31276166	0.58159875	5.23620613

H	-1.64407081	-2.73147093	2.88519066
H	-1.38905615	-1.97285643	4.47112875
H	-0.51802205	-3.47373696	4.05439701
H	2.65954418	-0.68094415	3.97764485
H	2.16041661	-2.24768297	4.67619335
H	1.34832282	-0.74375057	5.17737442
H	0.63820996	-2.77541200	0.76265385
H	1.68427057	-3.50481574	1.99634459
H	2.20860973	-2.03348969	1.14389137
H	0.56523253	1.92490697	-6.50771329
H	0.83323335	0.16580385	-6.28081836
H	2.06911751	1.17691906	-7.11523522
H	4.46608546	1.79588990	-3.83595045
H	4.16862059	2.48199135	-5.45351061
H	4.48895721	0.74224212	-5.27410860
H	4.29616604	-1.13307441	-1.90927454
H	5.04357203	-0.47304652	-3.38478038
H	5.04382200	-2.22976963	-3.09332885
H	2.08755803	-3.10471396	-2.00794817
H	2.59370131	-3.95094144	-3.50799492
H	0.98160220	-3.16028134	-3.41374916
H	1.96452439	-1.98250764	-6.05175518
H	3.62627388	-2.65939480	-5.86051251
H	3.40635146	-0.92940120	-6.22313996
H	0.48352505	3.19269109	-3.88228047
H	2.09814036	3.84007514	-4.25787033
H	1.81440114	2.99192722	-2.71645076
N	-0.73107994	1.48377987	-1.85939028
C	-1.68173429	2.41941731	-1.88388319
C	-0.45973015	0.82136397	-2.99165876
C	-2.42142205	2.71687930	-3.02649345
C	-1.18334066	1.00627107	-4.17351016
C	-2.17864732	1.97727844	-4.18340680
H	-1.86781417	2.94605173	-0.94370635
H	-3.18814613	3.49149848	-2.99233243
H	-2.76796322	2.15014312	-5.08629645
H	-0.92916578	0.33175589	-4.99823844
O	0.57620401	-0.97390525	-1.91312305
O	-0.00858042	-1.40923378	-4.81649806
C	0.67277560	-0.18636840	-2.85575755
C	-1.10572517	-2.18497108	-4.67370625
H	-2.06653651	-1.60428241	-4.54259237
H	-1.08097420	-2.86477960	-3.77870278
H	-1.31629866	-2.86698147	-5.54003730

H	0.60186306	3.34156678	4.27156678
H	1.71265335	2.64852342	3.05681311
H	1.44803971	1.80484137	4.59650776

Table S58. Atomic coordinates and single point energies for **60d**.



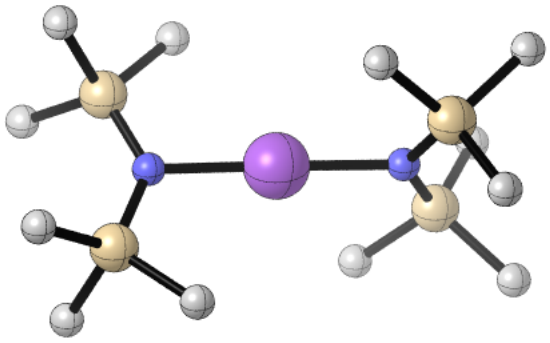
G = –2382.920174
G_{SP} = –2384.598272

Na	-1.61602000	0.12449400	-0.20279900
N	-3.81837600	-0.19030800	-0.03554800
N	2.50662300	-0.58295600	0.44319900
Si	-4.73691400	1.16225200	0.38665300
C	-3.64602600	2.72239600	0.29462800
C	-5.42862100	1.13264000	2.16085400
C	-6.23995200	1.49356600	-0.73581000
Si	-4.35638800	-1.76031500	-0.36959100
C	-2.89078300	-2.97110600	-0.35117700
C	-5.17056800	-1.95286300	-2.08061100
C	-5.63159600	-2.43948200	0.87308900
Si	3.05864300	-2.18199700	-0.20929000
C	2.64333300	-2.25817300	-2.02722800
C	2.20578200	-3.54938200	0.76695800
C	4.92355800	-2.23282000	-0.04192100
Si	3.42881500	0.27698100	1.72524600
C	2.36612800	1.66505600	2.43986800
C	5.09825100	0.91058400	1.17454700
C	3.59044800	-0.98589300	3.12225800
H	-2.79158000	2.63269900	0.98759900
H	-4.19655200	3.63817600	0.56241900
H	-3.24903000	2.85106500	-0.72626000
H	-5.92935300	1.55308900	-1.79085100
H	-6.75739800	2.43017700	-0.47177500

H	-6.96922500	0.67091200	-0.65138100
H	-4.47032200	-1.64459000	-2.87303400
H	-6.06196500	-1.31034500	-2.15916100
H	-5.47840100	-2.99244300	-2.27916100
H	-5.24161000	-2.37841300	1.90140900
H	-5.89204300	-3.48948200	0.66268100
H	-6.56157100	-1.84822700	0.83422200
H	-2.12987300	-2.69799400	-1.10142000
H	-3.20975300	-4.00255700	-0.57014800
H	-2.39846400	-2.97408400	0.63501600
H	5.26778400	1.92712000	1.56229200
H	5.11317000	0.91452200	0.06326700
H	5.90924500	0.26051100	1.53537900
H	2.59555200	-1.30685500	3.46719700
H	4.11792600	-0.52402500	3.97198500
H	4.15432900	-1.88134000	2.82510700
H	1.11651300	-3.44991200	0.64967800
H	2.44633900	-3.49682100	1.83915000
H	2.50741800	-4.54101700	0.39487200
H	1.56255800	-2.27142400	-2.21654000
H	3.10300100	-3.14994100	-2.48081200
H	3.10534300	-1.35329900	-2.45552500
H	5.27738300	-1.38017800	-0.64983600
H	5.29139700	-3.17372800	-0.48136300
H	5.31245800	-2.16244900	0.98343500
H	2.38275800	2.57755600	1.82810800
H	2.76977800	1.91344700	3.43479800
H	1.31694200	1.35725500	2.56810900
N	0.05461700	1.93210500	-0.14460600
C	-0.06931300	3.23712300	-0.38201100
C	1.25083200	1.37170600	-0.36527300
C	0.97710100	4.01421400	-0.88282000
C	2.35745300	2.03582700	-0.90393100
C	2.19277300	3.39710900	-1.16973300
H	-1.04818200	3.67948900	-0.17719200
H	0.81966300	5.07831800	-1.06418500
H	3.01624700	3.96975000	-1.60192900
H	3.29012900	1.42765500	-1.16598500
O	0.41106000	-0.83133600	-0.42969200
O	4.47091400	0.39231700	-1.72692800
C	1.35420500	-0.11165500	-0.09285100
C	4.78045600	0.83605300	-2.96758400
H	4.20839100	1.75884900	-3.28046800
H	4.56737800	0.10218800	-3.79184300

H	5.85616200	1.11915700	-3.11498600
H	-5.97559100	2.05731800	2.40769600
H	-4.60955600	1.01190200	2.88739900
H	-6.11598600	0.28249700	2.29471800

Table S59. Atomic coordinates and single point energies for **59**.

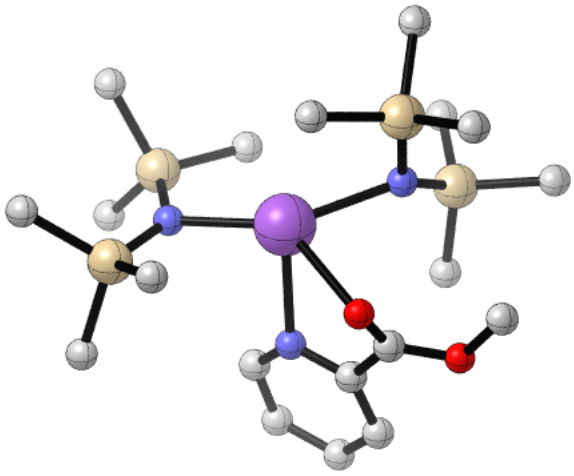


G = –1907.434448
G_{SP} = –1908.586391

Na	-0.00005400	0.02562500	-0.02609000
N	-2.23849600	0.00466100	-0.00301600
N	2.23860100	0.02092800	-0.02002500
Si	-2.97446200	1.06929100	-1.08559000
C	-1.67241000	1.75552700	-2.29429800
C	-3.77203700	2.59404700	-0.26826500
C	-4.34803400	0.29628900	-2.15727300
Si	-2.90541800	-1.08222700	1.10239300
C	-1.54170800	-1.72903700	2.26403000
C	-3.68412200	-2.62960900	0.30997000
C	-4.26347900	-0.35127600	2.22212600
Si	2.93564900	-1.09821500	-1.07314700
C	3.76574600	-0.32606500	-2.60405300
C	1.58928200	-2.26349200	-1.74924500
C	4.26650400	-2.21399900	-0.28796600
Si	2.94419400	1.11358300	1.05505500
C	1.62424600	2.33147500	1.68884900
C	4.34252000	2.17485200	0.31283700
C	3.69344000	0.31034000	2.61144000
H	-3.97064500	-0.59341800	-2.68562200
H	-4.73990700	1.00499100	-2.90500000
H	-5.19118000	-0.02636800	-1.52414200
H	-3.02026300	3.14537000	0.31855400
H	-4.57129300	2.28687000	0.42486300
H	-4.20697600	3.28468000	-1.00927800
H	-0.87876200	2.29854000	-1.75283400
H	-2.10849900	2.45673600	-3.02353800
H	-1.19497400	0.93754100	-2.85894100
H	-3.89490800	0.54971900	2.73740500

H	-4.60673600	-1.07131300	2.98280500
H	-5.13804600	-0.05473400	1.61961300
H	-0.75120500	-2.24924800	1.69611200
H	-1.93123900	-2.44213100	3.00793400
H	-1.06885000	-0.89735400	2.81247200
H	-2.93634000	-3.15718300	-0.30320000
H	-4.51554000	-2.34626800	-0.35491200
H	-4.07219000	-3.33388800	1.06404700
H	0.81761300	-1.69873600	-2.30016000
H	1.08883100	-2.80130300	-0.92675800
H	1.99845500	-3.01665900	-2.44130700
H	3.03829900	0.28511800	-3.16142000
H	4.17181700	-1.08971400	-3.28754800
H	4.59145400	0.33757600	-2.30173500
H	5.13343200	-1.61106600	0.02942700
H	4.62954300	-2.98346300	-0.98872300
H	3.86810500	-2.71846500	0.60642900
H	2.92366900	-0.26890700	3.14573500
H	4.10939600	1.05726600	3.30738100
H	4.49956400	-0.38802100	2.33565500
H	1.17343700	2.88837500	0.85074600
H	2.04055900	3.06714500	2.39535500
H	0.81277800	1.79804200	2.21322100
H	3.99385700	2.69313600	-0.59433300
H	5.19466700	1.53733000	0.02428700
H	4.71277100	2.93045300	1.02480500

Table S60. Atomic coordinates and single point energies for **60**.



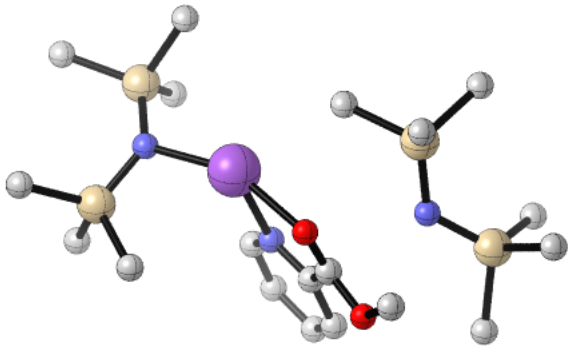
G = –2382.94305
G_{SP} = –2384.627751

Na	-0.27354000	-0.29085500	-0.50793800
N	-2.52497900	-0.51724300	-0.05604800
N	1.94552100	-0.83499700	0.04880400
Si	-3.50370800	0.00548800	-1.32234800
C	-4.98369200	-1.13158200	-1.71929400
C	-2.49679200	0.15391500	-2.92794700
C	-4.27773700	1.73251700	-1.04984200
Si	-2.84733300	-1.31757100	1.38907000
C	-1.23336300	-1.50562400	2.37316200
C	-3.55944800	-3.07492200	1.19781900
C	-4.07895800	-0.40958700	2.53579800
Si	2.17740400	-2.15592900	-0.98196900
C	0.63417300	-2.42664100	-2.06987700
C	2.50396800	-3.82046000	-0.11204200
C	3.60614600	-1.97944100	-2.23977200
Si	2.79028900	-0.49291300	1.47337700
C	2.35433200	1.22288100	2.16946000
C	4.69124300	-0.45957600	1.24882200
C	2.51434500	-1.70904400	2.91410700
H	-4.82033700	1.76677200	-0.09055200
H	-4.98561200	1.99650100	-1.85292800
H	-3.49525800	2.50826200	-1.02313900
H	-2.12462700	-0.83663500	-3.23644400
H	-1.62231400	0.81059800	-2.77977300
H	-3.09108200	0.56824200	-3.75848200
H	-4.63488400	-2.15682700	-1.92136000

H	-5.55335400	-0.78018400	-2.59528300
H	-5.67572100	-1.17930600	-0.86192800
H	-3.71573100	0.60223700	2.78045700
H	-4.24189100	-0.94898400	3.48334700
H	-5.05560300	-0.29905300	2.03581900
H	-0.49728500	-2.09193200	1.79691800
H	-1.37299300	-2.00499500	3.34551600
H	-0.77659900	-0.51857000	2.56227700
H	-2.87869100	-3.69000300	0.58786900
H	-4.53311500	-3.04733300	0.68319700
H	-3.69800900	-3.57526400	2.17035800
H	1.70315800	-4.03840400	0.61237400
H	3.45611000	-3.79109700	0.44326100
H	2.55721700	-4.65404400	-0.83127600
H	-0.26927200	-2.65338800	-1.47647300
H	0.78375200	-3.26886300	-2.76366700
H	0.43077500	-1.53384600	-2.68647000
H	3.38073600	-1.18546300	-2.96966500
H	3.76111100	-2.91652000	-2.79922600
H	4.55222800	-1.72406900	-1.73473000
H	1.45312900	-1.73174800	3.20511000
H	3.10926500	-1.42141400	3.79700500
H	2.80306200	-2.73211600	2.62631100
H	2.72412100	2.01152900	1.49598600
H	2.81265600	1.37517500	3.16010700
H	1.26338700	1.34873300	2.27605700
H	4.98841000	0.27567500	0.48344100
H	5.05874100	-1.44678700	0.92180700
H	5.21090500	-0.20196400	2.18653300
N	-0.47115300	2.03820900	-0.01460200
C	-1.32361200	2.50336300	0.89193600
C	0.63870100	2.71716000	-0.27723600
C	-1.10018600	3.70945900	1.56187100
C	0.96042800	3.92361700	0.34383400
C	0.05837200	4.42909400	1.27707100
H	-2.20026900	1.86983900	1.06980500
H	-1.82137500	4.06656500	2.29727700
H	0.26517600	5.37076600	1.78867300
H	1.89715700	4.42645500	0.10637900
O	1.13883800	1.28184000	-2.12077700
C	1.53568000	2.04992300	-1.28644800
O	2.80701000	2.40817100	-1.13595100
C	3.73992700	1.64135400	-1.89045000
H	4.73097800	2.03280800	-1.63960800

H	3.54136300	1.74294800	-2.96626500
H	3.64275000	0.58775800	-1.59418500

Table S61. Atomic coordinates and single point energies for **61**.

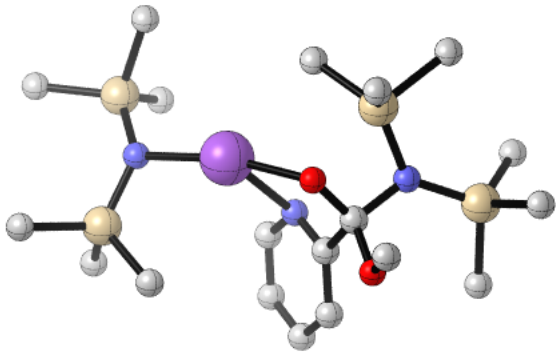


G = –2382.924637
G_{SP} = –2384.610658

Na	1.27275500	0.45142000	-0.94931600
N	3.43867800	0.42593800	-0.34222200
N	-2.96980700	0.40218700	0.07879200
Si	4.15186600	-1.02948100	-0.81352900
C	5.69986000	-0.84717600	-1.90934100
C	2.91532000	-2.05020600	-1.84500600
C	4.69168600	-2.16534000	0.62181300
Si	4.03234400	1.63095600	0.68304200
C	3.28458000	3.32361500	0.25591700
C	5.92486200	1.85837400	0.63749400
C	3.60201500	1.33370900	2.51774500
Si	-2.50955300	1.96964100	-0.32785800
C	-0.64937600	2.32234000	-0.00181500
C	-3.42035900	3.36116800	0.61354200
C	-2.75083800	2.39564500	-2.17421800
Si	-4.50176200	-0.07345600	0.58844900
C	-4.70412000	-1.96261900	0.76834200
C	-5.91847400	0.43030800	-0.60083400
C	-5.04139500	0.59277300	2.29432500
H	5.42600900	-1.65088700	1.26346800
H	5.15352900	-3.09878600	0.26062900
H	3.82886300	-2.43438500	1.25219900
H	2.58349500	-1.48787600	-2.73476200
H	2.02182800	-2.30860800	-1.25246600
H	3.36083200	-2.99237800	-2.20177000
H	5.47038800	-0.23079700	-2.79287900
H	6.07474400	-1.82402900	-2.25639000
H	6.51092800	-0.34645400	-1.35757800
H	2.50782500	1.33228600	2.65392400

H	4.02198600	2.10735500	3.18104800
H	3.98543100	0.35438300	2.84948200
H	3.54260300	3.60682500	-0.77698000
H	3.64408500	4.11738100	0.93023000
H	2.18492500	3.29411200	0.33144900
H	6.26128600	2.09368800	-0.38479200
H	6.43879900	0.93504200	0.95258200
H	6.25404700	2.67189500	1.30423800
H	-3.25295500	3.26785500	1.69861900
H	-4.50804700	3.31612600	0.43963100
H	-3.06730000	4.35630700	0.29598700
H	-0.22095200	1.53136800	0.63457300
H	-0.50457800	3.28149200	0.51866000
H	-0.09822500	2.39866000	-0.95519500
H	-2.14169600	1.71507400	-2.79073300
H	-2.45158400	3.43134700	-2.40617500
H	-3.80662600	2.27051700	-2.46706100
H	-4.28147600	0.34006000	3.05110100
H	-6.00498600	0.16270100	2.61489200
H	-5.14382900	1.68891400	2.28053200
H	-4.37054500	-2.49584900	-0.13579700
H	-5.76308600	-2.21057600	0.94758500
H	-4.12494200	-2.33897200	1.62661200
H	-5.77038400	-0.01879700	-1.59704000
H	-5.94054600	1.52448800	-0.73496600
H	-6.90826700	0.11478000	-0.23087400
N	0.37839100	-1.08500000	0.58933900
C	0.94626500	-1.45823200	1.73218400
C	-0.75097400	-1.66890200	0.19901000
C	0.39762700	-2.45165400	2.54347500
C	-1.36646800	-2.68674900	0.92747300
C	-0.77733400	-3.07555000	2.12648000
H	1.87913100	-0.94693400	1.99086900
H	0.89003400	-2.73032700	3.47520700
H	-1.23274400	-3.86130400	2.73193200
H	-2.28502000	-3.13439400	0.55519700
O	-0.69089100	-0.37680000	-1.81054900
C	-1.27467600	-1.19668300	-1.13039400
O	-2.30110600	-1.91040500	-1.56063500
C	-2.98828400	-1.37268400	-2.67924200
H	-3.82117900	-2.05368400	-2.88485400
H	-2.31925300	-1.30356000	-3.54806200
H	-3.35775400	-0.37398200	-2.40484200

Table S62. Atomic coordinates and single point energies for **62**.

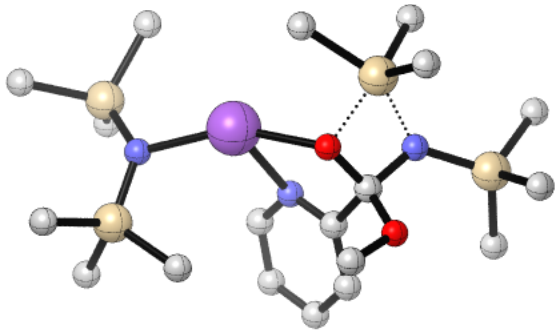


G = –2382.945822
G_{SP} = –2384.624228

Na	-1.02570000	0.62779700	0.75492500
N	-3.22785800	0.45699200	0.31984600
N	2.74307600	0.27276600	-0.05691700
Si	-3.81581200	-1.02548600	0.87567700
C	-5.22317100	-0.88878600	2.15350600
C	-2.42690900	-1.99442300	1.74655200
C	-4.49682300	-2.18026600	-0.48364600
Si	-3.97241000	1.54423000	-0.73687100
C	-3.31254700	3.31030200	-0.50280100
C	-5.86692700	1.66781200	-0.54648500
C	-3.66981500	1.13113900	-2.57526400
Si	2.25230700	1.91349100	0.48698100
C	0.62466600	2.69658300	-0.12857900
C	3.48604700	2.98180600	-0.56850000
C	2.72710000	2.56975500	2.21032400
Si	4.16240000	-0.32085800	-0.87895600
C	4.05291700	-2.18121300	-1.17558500
C	5.73664900	-0.03998100	0.13673200
C	4.40674600	0.47087000	-2.57683000
H	-5.35593000	-1.71239700	-0.99231700
H	-4.83099700	-3.14870500	-0.07657000
H	-3.72543200	-2.37582000	-1.24528300
H	-2.00298600	-1.41506200	2.58468600
H	-1.60326400	-2.23822400	1.05443000
H	-2.79529600	-2.94562300	2.16304800
H	-4.90053200	-0.27549100	3.00965200
H	-5.53633700	-1.87550500	2.53251300
H	-6.10264600	-0.39827900	1.70697800
H	-2.59107700	1.18441100	-2.79821400

H	-4.18979300	1.82263400	-3.25835700
H	-4.01018000	0.10654300	-2.79877600
H	-3.48430100	3.64979600	0.53110500
H	-3.80246100	4.02381400	-1.18496500
H	-2.22802900	3.35484300	-0.69440600
H	-6.12946700	1.97249700	0.47926000
H	-6.34617100	0.69308200	-0.73598700
H	-6.30272300	2.40026200	-1.24542300
H	3.25980600	2.91870600	-1.64554800
H	4.54940500	2.71981300	-0.43318100
H	3.37519100	4.03955300	-0.27519300
H	0.15990000	2.04361500	-0.88643600
H	0.78644000	3.67896600	-0.59583300
H	-0.08171200	2.85100900	0.70474300
H	2.06928400	2.17796900	2.99771000
H	2.67374800	3.67086800	2.20929700
H	3.76759600	2.29989300	2.45606000
H	3.45235500	0.49025600	-3.12478700
H	5.12689000	-0.12686500	-3.15845200
H	4.78531400	1.49954500	-2.51399300
H	3.91101600	-2.71368700	-0.22479400
H	4.99514400	-2.52204100	-1.63443000
H	3.22555000	-2.44638400	-1.85023500
H	5.73236600	-0.68756800	1.02715200
H	5.81197700	1.00364400	0.47772400
H	6.63732000	-0.27533200	-0.45272600
N	-0.00678700	-0.81759500	-0.87171800
C	-0.84416800	-1.52894700	-1.62453900
C	0.91888100	-1.44511100	-0.14132500
C	-0.79450400	-2.91960100	-1.70392700
C	1.01752600	-2.84144200	-0.12863700
C	0.15421500	-3.58282900	-0.92902400
H	-1.61177500	-0.96321100	-2.16173800
H	-1.50374600	-3.46040400	-2.33086200
H	0.21010100	-4.67345400	-0.93462800
H	1.75434900	-3.31203900	0.51744500
O	1.08328500	0.41251200	1.37133600
C	1.80827400	-0.52671000	0.72717500
O	2.48674700	-1.43190900	1.60177900
C	3.10384100	-0.82052400	2.69887900
H	3.61303800	-1.61170200	3.26675200
H	2.36724300	-0.31614400	3.34215500
H	3.85146300	-0.07339300	2.38106800

Table S63. Atomic coordinates and single point energies for **TS-6**.

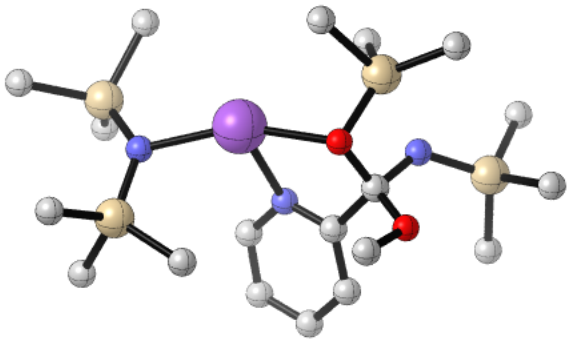


G = –2382.935844
G_{SP} = –2384.615248

Na	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.25727897
N	1.85971739	0.00000000	-3.44115119
Si	0.42054201	1.49547195	2.91781903
C	-1.00845443	2.38271059	3.81434478
C	0.98790022	2.69737121	1.55217839
C	1.84636063	1.43879204	4.18402821
Si	-0.31037039	-1.47254159	3.01934745
C	-1.03697705	-2.71254086	1.77300952
C	-1.53843589	-1.37939495	4.47442761
C	1.23510704	-2.33626028	3.73410354
Si	0.04033808	-0.54655478	-3.29322195
C	-1.43296439	-1.06070627	-2.10433669
C	0.37505243	-2.36685256	-3.82762730
C	-0.81671095	0.32472551	-4.75008734
Si	2.97238608	0.13769558	-4.76740958
C	4.69601025	0.66765880	-4.18719142
C	2.45885790	1.39085476	-6.09042977
C	3.19020244	-1.52008959	-5.65030839
H	1.55286735	0.85535197	5.07238953
H	2.13756091	2.44652895	4.52272078
H	2.73278189	0.95412837	3.74386064
H	0.24627165	2.75761406	0.73671407
H	1.94697717	2.37788381	1.11154692
H	1.12429240	3.71773923	1.94562853
H	-1.85257637	2.53578033	3.12332780
H	-0.70463058	3.36532585	4.21115350
H	-1.37684065	1.77214624	4.65399439
H	1.93633044	-2.60740266	2.92805193
H	0.97518355	-3.26088401	4.27535094

H	1.76802842	-1.67002152	4.43110333
H	-1.96843005	-2.32513094	1.32891473
H	-1.26209516	-3.68630995	2.23656159
H	-0.32332826	-2.89835069	0.95172481
H	-2.47377592	-0.89086135	4.15879574
H	-1.11317418	-0.78132699	5.29747341
H	-1.78428354	-2.37654046	4.87458510
H	0.91841854	-2.88859821	-3.02099311
H	0.99134817	-2.44310551	-4.73322395
H	-0.56678225	-2.91267504	-4.00012497
H	-1.11888153	-1.76082110	-1.30669837
H	-2.18844916	-1.61342221	-2.68488803
H	-1.94430809	-0.19735075	-1.64238325
H	-0.62990591	1.40826106	-4.69360502
H	-1.90489167	0.15739303	-4.76263609
H	-0.40763881	-0.03779064	-5.70705047
H	3.36590913	-2.33971943	-4.93842694
H	4.05796606	-1.45017461	-6.32585193
H	2.31266073	-1.77895881	-6.26055634
H	4.70571608	1.73209216	-3.91161789
H	5.41795282	0.52712412	-5.00777574
H	5.03668838	0.08257623	-3.31967766
H	2.34725054	2.37911294	-5.62191337
H	1.49233591	1.11962576	-6.54046614
H	3.21073950	1.45418458	-6.89401314
N	2.34974367	0.00631140	-0.33632097
C	3.14061108	-0.15116573	0.72400635
C	2.66649570	0.90799660	-1.26754159
C	4.31421938	0.57770116	0.90579201
C	3.81310338	1.70293969	-1.15514214
C	4.64875021	1.52763894	-0.05740134
H	2.79641286	-0.86256131	1.48046001
H	4.92743150	0.41930393	1.79302300
H	5.54642743	2.13930399	0.05462736
H	4.01647246	2.45145413	-1.91875930
O	0.39919479	0.81444546	-2.04947738
C	1.69264245	1.02765964	-2.46370150
O	1.87046339	2.31504089	-3.05100883
C	1.28735456	3.37186669	-2.33563274
H	1.52887567	4.30018468	-2.87139720
H	1.68073548	3.44373370	-1.30477612
H	0.19458346	3.25447692	-2.27675587

Table S64. Atomic coordinates and single point energies for **63**.

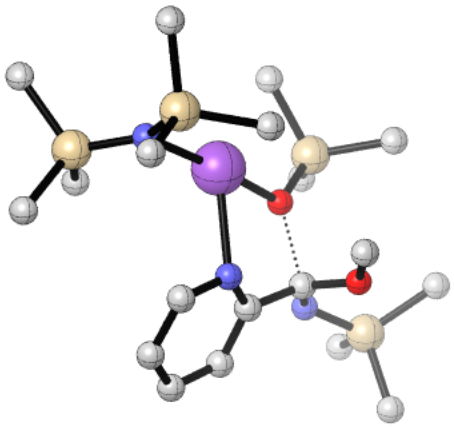


G = –2382.938755
G_{SP} = –2384.618939

Na	-1.00743900	0.86854100	0.58104700
N	-3.17332200	0.37344600	0.22515700
N	2.82052200	0.29787800	-0.15329900
Si	-3.66893500	-1.07637700	0.93341500
C	-4.96182200	-0.86384500	2.31700700
C	-2.19302100	-1.96962700	1.74462300
C	-4.43773000	-2.33592200	-0.27639000
Si	-3.98974500	1.40225700	-0.83351400
C	-3.09320000	3.07721200	-0.93842300
C	-5.79397800	1.78202200	-0.35127600
C	-4.07312900	0.76548800	-2.63109600
Si	2.02538400	1.97924100	0.53069600
C	0.74189200	3.14448700	1.46544700
C	1.71427800	2.65822800	-1.22040600
C	3.60647900	2.59597900	1.39138900
Si	4.37654600	-0.21326300	-0.67414800
C	4.35559600	-1.88539500	-1.56969000
C	5.65403200	-0.38984300	0.71473600
C	5.02831800	1.06155000	-1.90958200
H	-5.35138500	-1.92253600	-0.73488700
H	-4.70836000	-3.27885500	0.22629000
H	-3.73271900	-2.57156300	-1.08983400
H	-1.64739500	-1.29636800	2.42856500
H	-1.47802400	-2.33353800	0.98783100
H	-2.52442600	-2.83799300	2.33666400
H	-4.56775700	-0.20515100	3.10707000
H	-5.24296100	-1.82546700	2.77683400
H	-5.87514800	-0.39265500	1.92018600
H	-3.06212700	0.71592900	-3.06778200

H	-4.68404500	1.41824000	-3.27600500
H	-4.50340000	-0.24854500	-2.66410600
H	-3.05220300	3.55969900	0.05157100
H	-3.58964200	3.77265100	-1.63392300
H	-2.05584500	2.94884200	-1.29404100
H	-5.84235800	2.17511500	0.67652400
H	-6.40198300	0.86263900	-0.38385600
H	-6.25869600	2.51800600	-1.02735800
H	0.89691400	2.06616000	-1.66891400
H	2.59154200	2.51402200	-1.86704900
H	1.41590400	3.71807400	-1.22873800
H	-0.28666200	3.14385700	1.05199100
H	1.07442800	4.19328000	1.38885700
H	0.66439200	2.89764500	2.53830600
H	3.80658600	1.92746300	2.24538800
H	3.52134200	3.62542500	1.77027300
H	4.47916400	2.53436700	0.72338700
H	4.39213100	1.08544700	-2.80760000
H	6.05566800	0.81189800	-2.21899700
H	5.03841200	2.07443400	-1.47944500
H	4.22267000	-2.71750200	-0.86206800
H	5.31462800	-2.04101000	-2.09028400
H	3.54449100	-1.93364800	-2.31216200
H	5.25775400	-1.08649600	1.46848400
H	5.83603700	0.57425500	1.21229800
H	6.61555700	-0.77617700	0.33918300
N	-0.06849500	-0.79008800	-0.83556600
C	-0.86646300	-1.51916300	-1.61521200
C	0.99000500	-1.36082700	-0.25846700
C	-0.63785500	-2.86827000	-1.87621300
C	1.28335900	-2.71749600	-0.44319600
C	0.46071700	-3.47542000	-1.26860900
H	-1.74746800	-1.00617500	-2.01306200
H	-1.32044700	-3.42724500	-2.51652300
H	0.66577300	-4.53631600	-1.42679200
H	2.13848700	-3.14919100	0.07501800
O	1.12544300	0.55991000	1.18756500
C	1.89216300	-0.44674100	0.59980100
O	2.53658900	-1.24736500	1.58348700
C	1.70625300	-1.68827700	2.62485600
H	2.31466200	-2.32712500	3.27949200
H	0.84758800	-2.27798500	2.25374500
H	1.31269600	-0.83971800	3.20542100

Table S65. Atomic coordinates and single point energies for **TS-7**.



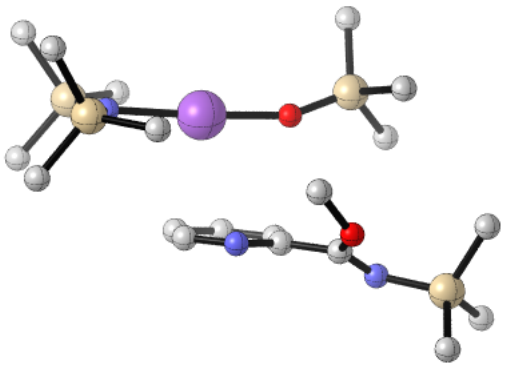
G = –2382.923189
G_{SP} = –2384.608706

Na	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.25785438
N	2.04738534	0.00000000	-3.98618119
Si	-0.77052281	1.36071838	2.87807755
C	-2.40223692	1.01281356	3.79574723
C	-1.21576812	2.52596710	1.43507905
C	0.27409849	2.39740985	4.09025339
Si	0.86344545	-1.29429335	2.90297355
C	1.47471410	-2.41007428	1.48596906
C	-0.13516835	-2.41130986	4.07882419
C	2.42606521	-0.80997132	3.88516681
Si	-1.07283141	-0.74132370	-3.04627947
C	-2.24340732	-1.61347077	-1.82723079
C	-0.54462315	-2.04266244	-4.30778913
C	-2.07420585	0.61707401	-3.90263849
Si	2.06998562	0.39275829	-5.64879500
C	3.38065935	1.73014345	-5.95569222
C	0.48101467	1.03784997	-6.46054967
C	2.60341109	-1.15156868	-6.60078512
H	0.48443517	1.82093016	5.00573617
H	-0.23967097	3.32641500	4.38681555
H	1.24253293	2.66936607	3.64063054
H	-1.90711175	2.03138656	0.72952049
H	-0.30597863	2.80597247	0.87695255
H	-1.70517981	3.45384079	1.77091964
H	-3.10076864	0.47070450	3.13906891
H	-2.89483221	1.93825988	4.13629849

H	-2.21911884	0.37806662	4.67749588
H	3.13588001	-0.26424131	3.24304765
H	2.94499575	-1.69674602	4.28468633
H	2.16991466	-0.15415756	4.73250197
H	0.62534202	-2.80768747	0.90481409
H	2.05514458	-3.27192457	1.85173099
H	2.12304044	-1.84682453	0.79197321
H	-1.05371451	-2.76295394	3.58332218
H	-0.43865516	-1.84720715	4.97584441
H	0.44032572	-3.29136752	4.40925833
H	0.18451569	-2.72504788	-3.84568656
H	-0.05785777	-1.59091763	-5.18216095
H	-1.41168291	-2.62836595	-4.65340846
H	-1.72119379	-2.42781237	-1.29897524
H	-3.11500019	-2.05238023	-2.33873932
H	-2.62967761	-0.91084231	-1.06912749
H	-2.61825620	1.21197850	-3.15125028
H	-2.80791802	0.21649898	-4.62011923
H	-1.39314456	1.29348813	-4.43903199
H	3.56635070	-1.51504475	-6.21067493
H	2.71809452	-0.94546531	-7.67671895
H	1.87126063	-1.96439228	-6.48035513
H	3.11257694	2.63455189	-5.38786981
H	3.46613824	1.99820818	-7.02093829
H	4.36776869	1.39098290	-5.60443575
H	0.19096488	1.99172905	-5.99494376
H	-0.36340743	0.34030600	-6.35725383
H	0.65162048	1.21121020	-7.53584008
N	2.03276577	1.05033268	-0.53478335
C	2.85282924	1.09032188	0.51746409
C	2.51231958	0.71428824	-1.73478908
C	4.21296214	0.80622934	0.42789268
C	3.86676219	0.40212231	-1.91324542
C	4.72319921	0.45089325	-0.81971072
H	2.38048232	1.32506597	1.47757058
H	4.84211227	0.84554636	1.31763750
H	5.78068537	0.20479890	-0.93752672
H	4.19214751	0.10899297	-2.90984608
O	0.14596899	-0.10376623	-2.15814692
C	1.62478409	0.70281844	-2.98957295
O	1.06115954	1.93642171	-3.30086702
C	0.43336570	2.74578597	-2.33969306
H	-0.02627137	3.57677299	-2.89281977
H	1.14447179	3.15573305	-1.60564107

H	-0.34865511	2.18917807	-1.80490934

Table S66. Atomic coordinates and single point energies for **64**.

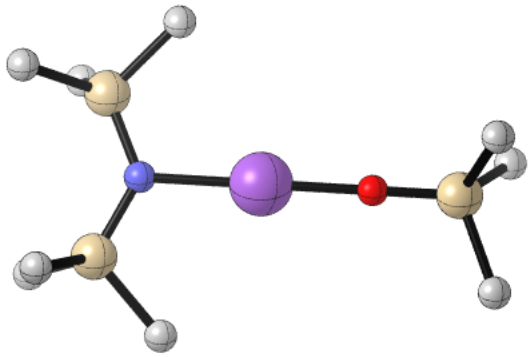


G = –2382.943615
G_{SP} = –2384.634413

Na	-1.50201900	-0.75620600	-0.21497000
N	-3.61482100	0.03959500	-0.16034100
N	3.72862300	0.88818000	0.92705400
Si	-3.89327800	1.12478900	-1.42108100
C	-5.20372600	0.56617700	-2.68556200
C	-2.28701000	1.36740300	-2.41742600
C	-4.45372600	2.86370300	-0.87273100
Si	-4.59295000	-0.57339300	1.06576200
C	-3.61970000	-1.86084400	2.07995400
C	-6.16839000	-1.46702000	0.47504000
C	-5.21816800	0.72196900	2.32092500
Si	1.57487300	-2.59050600	-0.68603600
C	0.87402300	-4.34689700	-0.90741800
C	2.77970500	-2.69897700	0.78574200
C	2.66111600	-2.25774400	-2.21330500
Si	5.37399400	0.91731900	0.32672300
C	5.80743100	2.67284200	-0.20504900
C	5.66187100	-0.27450800	-1.10013600
C	6.46601600	0.41124600	1.77345300
H	-5.44716900	2.81162700	-0.39833700
H	-4.52240700	3.55999900	-1.72438800
H	-3.76112600	3.29561300	-0.13284000
H	-1.95783000	0.41279300	-2.86315200
H	-1.46318600	1.74162400	-1.78602300
H	-2.42197900	2.08345300	-3.24378000
H	-4.94746600	-0.42732200	-3.08600500
H	-5.28846900	1.26876000	-3.53068800
H	-6.19408700	0.48508100	-2.20972000
H	-4.38710400	1.29632200	2.76052700

H	-5.78399400	0.25562300	3.14404800
H	-5.88230300	1.44537600	1.82130000
H	-3.30525300	-2.70033800	1.43727100
H	-4.21856900	-2.28049700	2.90390600
H	-2.70933600	-1.42148500	2.52152800
H	-5.91414200	-2.24657800	-0.26022300
H	-6.85313100	-0.75820800	-0.01796500
H	-6.71312400	-1.94005800	1.30845400
H	2.23662600	-2.94080400	1.71423900
H	3.29912800	-1.73862000	0.93986800
H	3.54243900	-3.47961300	0.62716700
H	0.27729200	-4.63730600	-0.02767000
H	1.66867800	-5.09865700	-1.04273600
H	0.21136200	-4.38853200	-1.78665200
H	2.04442100	-2.22233300	-3.12606900
H	3.43856300	-3.02684900	-2.35289400
H	3.16479900	-1.28359400	-2.11090800
H	6.30627500	1.08454500	2.62881800
H	7.53359600	0.43263100	1.50579200
H	6.21125000	-0.60934100	2.09758100
H	5.15052800	2.97776500	-1.03290200
H	6.85358400	2.74718600	-0.54001300
H	5.65945300	3.37720200	0.62712700
H	5.12000800	0.06236700	-1.99526100
H	5.29824200	-1.28188700	-0.84640500
H	6.73481700	-0.34296500	-1.33985600
N	0.37072600	1.79661200	0.37798600
C	-0.80819600	1.81293500	1.00017000
C	1.33909600	1.03798200	0.88729200
C	-1.07649100	1.07031300	2.14957300
C	1.18511600	0.28354700	2.05593200
C	-0.04974300	0.29408300	2.68940600
H	-1.59574800	2.42719200	0.55353600
H	-2.07473400	1.09513300	2.58741600
H	-0.21907300	-0.30610000	3.58531800
H	2.02893600	-0.30092100	2.41795900
O	0.43439400	-1.47388300	-0.50250000
C	2.68876700	1.04540000	0.22109500
O	2.77297400	1.28222400	-1.09954700
C	1.68447300	1.08593900	-2.00644700
H	2.15161700	0.85836200	-2.97375800
H	1.08312900	1.99936000	-2.08063700
H	1.06533200	0.23458500	-1.68301900

Table S67. Atomic coordinates and single point energies for **65**.

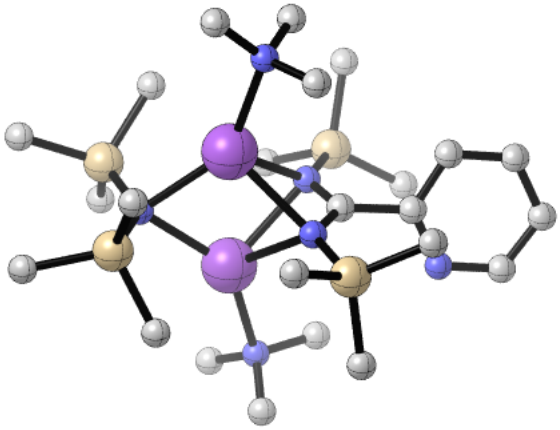


G = –1518.978897
G_{SP} = –1519.921239

Na	-0.59574800	0.00011900	-0.00044700
N	1.65812400	0.00014500	-0.00055900
Si	2.38505400	1.52381900	-0.00437400
C	3.15464600	2.03322500	1.66358200
C	1.09218700	2.86352600	-0.39989100
C	3.78302100	1.73952100	-1.28345800
Si	2.38406300	-1.52395000	0.00433500
C	1.08846900	-2.86324600	0.39258800
C	3.77653100	-1.74217100	1.28897500
C	3.16013200	-2.03228300	-1.66096100
Si	-4.25163600	-0.00007600	0.00020300
C	-5.01075500	-0.85800700	1.52481500
C	-5.00834700	-0.89093900	-1.50675500
C	-5.00988800	1.74947500	-0.01933700
H	4.62664800	1.06974300	-1.04747800
H	4.16887700	2.77182700	-1.30569600
H	3.42616400	1.48020400	-2.29279200
H	0.28084200	2.86544300	0.34759200
H	0.63626700	2.68727200	-1.38780900
H	1.53271400	3.87332700	-0.40761800
H	2.39255700	2.00210000	2.45835800
H	3.57933600	3.05012100	1.63219000
H	3.95747400	1.33496400	1.94896700
H	2.40128900	-1.99975800	-2.45878600
H	3.58375500	-3.04959400	-1.62872700
H	3.96475700	-1.33452400	-1.94244500
H	0.62750100	-2.68758700	1.37827500
H	1.52839600	-3.87329400	0.40169700
H	0.28119600	-2.86389100	-0.35930200

H	3.41565100	-1.48358500	2.29706700
H	4.62159300	-1.07272500	1.05721200
H	4.16158200	-2.77476600	1.31181400
H	-4.67991200	-1.94217700	-1.53785900
H	-4.67653500	-0.41329000	-2.44255400
H	-6.11068900	-0.87759100	-1.48838100
H	-4.68153000	-1.90799500	1.57989800
H	-6.11307700	-0.84586900	1.50404000
H	-4.68113100	-0.35957100	2.45050100
H	-4.68086000	2.32154500	0.86292000
H	-6.11222700	1.72618000	-0.02001200
H	-4.67919500	2.30234800	-0.91313200
O	-2.65322200	0.00089100	0.00140500

Table S68. Atomic coordinates and single point energies for **66**.



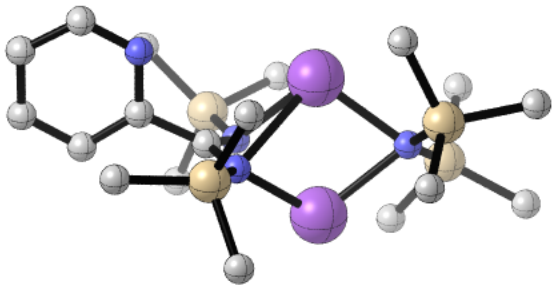
G = –2758.058575
G_{SP} = –2760.017343

N	3.61642700	0.76188800	-0.66415300
C	4.94867400	0.75874800	-0.65356300
C	2.97814600	-0.13862500	0.08376400
C	5.70883900	-0.15200300	0.07909500
C	3.64919600	-1.08866600	0.86298300
C	5.03894700	-1.10132800	0.84982100
H	5.44087600	1.51890500	-1.26744700
H	6.79751100	-0.11572600	0.04160700
H	5.59434300	-1.83695200	1.43405500
H	3.07832800	-1.80146500	1.46103200
C	1.46435700	-0.10596300	0.05378900
N	0.83246700	-0.52773000	-1.03017700
N	0.81441200	0.34018000	1.12020900
Si	1.52094000	-1.10604500	-2.53233000
C	3.09681800	-2.14327800	-2.35728100
C	1.88879400	0.32985900	-3.69797500
C	0.25312200	-2.20946200	-3.38355300
Si	1.42674500	1.07090700	2.58187700
C	0.15364300	2.34204400	3.14355400
C	3.09288600	1.95613500	2.42248200
C	1.59122200	-0.19250500	3.97704800
H	3.13683700	2.59669500	1.52945100
H	3.93587900	1.25135000	2.36450300
H	3.24601100	2.59245200	3.30857800
H	0.63334500	-0.69826900	4.17187000
H	1.89872500	0.31369200	4.90553200
H	2.34882500	-0.95858300	3.74994300

H	-0.00081500	3.13136500	2.39075100
H	0.47930100	2.83101300	4.07471600
H	-0.82183400	1.86960000	3.33195500
H	3.97751700	-1.54822100	-2.07418600
H	3.30998900	-2.61576200	-3.32957600
H	2.97940900	-2.95028600	-1.61724800
H	2.53715600	1.06575800	-3.19910700
H	0.95702100	0.82593400	-4.01059300
H	2.39749200	-0.02642400	-4.60724900
H	0.07082700	-3.14069100	-2.82637600
H	0.62342000	-2.48854400	-4.38257000
H	-0.71224300	-1.69868800	-3.50975700
Na	-0.96226600	-1.23835000	0.46764400
N	-2.71550300	0.19864300	-0.08446800
Na	-0.74111100	1.34377100	-0.51038200
Si	-3.29337600	-0.32861500	-1.59253800
C	-2.32619800	0.56488400	-2.96996300
C	-5.12506200	-0.02528400	-1.96123600
C	-3.01417800	-2.20380400	-1.79571500
Si	-3.47776100	0.50045700	1.40407800
C	-2.55932100	-0.47012200	2.77314400
C	-5.29114700	-0.03223600	1.53852500
C	-3.42127200	2.33844700	1.86830700
H	-2.56398800	1.64195400	-2.93546700
H	-2.58200500	0.20096800	-3.97731700
H	-1.23568400	0.44506900	-2.84870300
H	-1.96050500	-2.47788400	-1.61307300
H	-3.27495300	-2.58145100	-2.79691300
H	-3.63760500	-2.73589300	-1.05735600
H	-5.38445400	1.03497800	-1.81324700
H	-5.77240600	-0.62496600	-1.30408200
H	-5.36173000	-0.29127300	-3.00362100
H	-5.41237300	-1.09679600	1.28081100
H	-5.93055300	0.55232300	0.85975000
H	-5.66557400	0.11327000	2.56421400
H	-2.70773200	-1.55400800	2.61657500
H	-2.92608200	-0.23420000	3.78411900
H	-1.47514000	-0.26223400	2.75800900
H	-2.39406700	2.73130600	1.80742300
H	-3.79517100	2.53531500	2.88534200
H	-4.04050600	2.91182100	1.15960900
N	0.02371900	3.50797300	-1.16567400
C	1.33116400	3.59530400	-0.52769700
H	1.97177300	2.75677200	-0.84542400

H	1.21437400	3.54354800	0.56403600
H	1.84399000	4.54830000	-0.77404900
C	-0.88002200	4.53137600	-0.66300900
H	-0.51191500	5.55335400	-0.88884000
H	-0.98991600	4.43747000	0.42691500
H	-1.87367100	4.41103000	-1.11826400
C	0.15530300	3.59834400	-2.61226600
H	0.82831000	2.80961500	-2.97350900
H	0.56942200	4.58000000	-2.92240000
H	-0.82461700	3.46811000	-3.09254000
N	-0.44184100	-3.44902400	1.18031500
C	-1.54189500	-4.39800100	1.24709500
H	-2.31617400	-4.02635400	1.93329900
H	-1.20688100	-5.39323000	1.60490000
H	-1.99167000	-4.51726000	0.25156000
C	0.14329800	-3.21777400	2.49182900
H	0.60974600	-4.13505500	2.90692600
H	-0.62936500	-2.87101000	3.19303300
H	0.91012700	-2.43162800	2.42211800
C	0.57240500	-3.88299600	0.23216200
H	0.12037800	-4.02582200	-0.75954900
H	1.04793100	-4.83667500	0.54164800
H	1.35213800	-3.11219400	0.13865900

Table S69. Atomic coordinates and single point energies for **66a**.

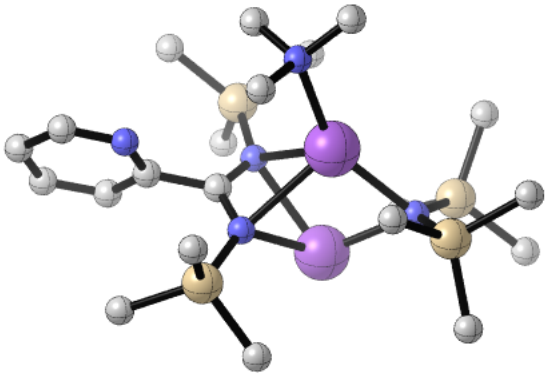


G = –2409.743596
G_{SP} = –2411.307627

N	-3.07289800	-0.25430100	1.40334600
C	-4.31053200	-0.27207900	1.89715600
C	-2.91694100	0.06613900	0.11707500
C	-5.44380400	0.01467300	1.13653000
C	-3.98516000	0.37831300	-0.72890400
C	-5.27343500	0.34435800	-0.20733200
H	-4.40809700	-0.53145500	2.95538100
H	-6.43370100	-0.02155600	1.59115600
H	-6.13486700	0.57189700	-0.83758600
H	-3.79646400	0.63253400	-1.77324100
C	-1.48536900	0.07566700	-0.36239900
N	-0.90138900	-1.06704500	-0.66698600
N	-0.81968700	1.22542600	-0.35475800
Si	-1.52974500	-2.69553900	-0.75552500
C	-3.40613900	-2.87383300	-0.88880000
C	-0.96352900	-3.67599500	0.74924000
C	-0.80956700	-3.45958000	-2.32155700
Si	-1.34915900	2.85868600	-0.04244800
C	0.10556700	3.74875600	0.76076600
C	-2.80024000	3.05566900	1.15304300
C	-1.77093900	3.70447300	-1.67249000
H	-2.60873400	2.51724900	2.09403800
H	-3.75491100	2.69158800	0.74712200
H	-2.91915500	4.12420800	1.39323800
H	-0.91862400	3.65583100	-2.36715400
H	-2.02596700	4.76414800	-1.51936100
H	-2.63064200	3.21583600	-2.15624000
H	0.33493300	3.31185400	1.74739900
H	-0.12982300	4.81144700	0.92588700
H	1.01757000	3.69547900	0.14874500
H	-3.93674300	-2.52400700	0.00942600

H	-3.64014600	-3.94202600	-1.02425200
H	-3.80834900	-2.33077300	-1.75720600
H	-1.33269300	-3.20179000	1.67228300
H	0.13341500	-3.73806200	0.80387100
H	-1.35806500	-4.70322000	0.71442700
H	-1.16830500	-2.91539100	-3.20935900
H	-1.11653500	-4.51144400	-2.42634700
H	0.29028000	-3.43185200	-2.32579000
Na	0.95485900	0.02642700	-1.57968700
N	2.59544000	-0.06856300	0.05731000
Na	0.58331500	0.12203200	1.19814600
Si	3.10309100	-1.54135200	0.75756000
C	2.80493000	-3.00753500	-0.40093400
C	2.05801200	-1.88997900	2.32835200
C	4.90440200	-1.62406400	1.33000700
Si	3.54273600	1.28878700	-0.36454500
C	2.66531600	2.21323200	-1.79335300
C	5.27593700	0.90972100	-1.03125300
C	3.78033000	2.51990400	1.05568300
H	1.75634800	-3.00671000	-0.73911400
H	3.00601600	-3.97970600	0.07551200
H	3.44704100	-2.92558000	-1.29252000
H	5.59218700	-1.62203000	0.47124900
H	5.08564800	-2.54693500	1.90286800
H	5.16415500	-0.76825500	1.97323200
H	0.98400300	-2.05284600	2.12450700
H	2.16637400	-1.07313900	3.06416200
H	2.39879400	-2.80981100	2.82799200
H	5.24460700	0.11031900	-1.78875000
H	5.95654800	0.58775800	-0.22927400
H	5.71388500	1.80532700	-1.49991000
H	2.71370000	1.62603900	-2.72933600
H	3.16138600	3.17162000	-2.00994100
H	1.60906600	2.44340100	-1.57092700
H	2.81800900	2.85057900	1.47524100
H	4.33806400	3.41602100	0.74152200
H	4.34966300	2.03661400	1.86606200

Table S70. Atomic coordinates and single point energies for **66b**.



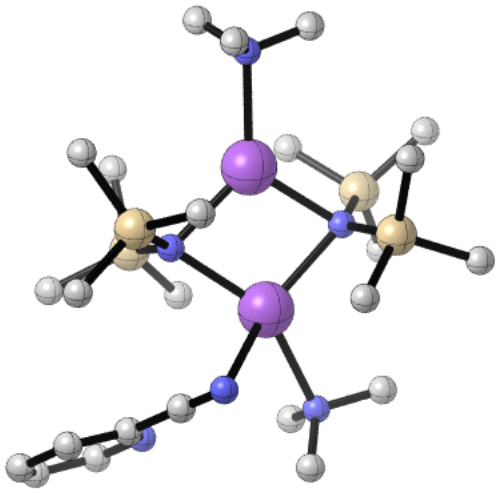
G = –2583.904557
G_{SP} = -2585.665658

N	-3.51207000	-0.51215800	0.64891400
C	-4.83927700	-0.55680100	0.76270100
C	-2.99180300	0.07279500	-0.43106400
C	-5.70939300	-0.04832700	-0.20055300
C	-3.77887000	0.62563600	-1.44761400
C	-5.16202500	0.55187200	-1.33386800
H	-5.23319700	-1.03038300	1.66684100
H	-6.78784300	-0.12526800	-0.06271500
H	-5.80674300	0.95680900	-2.11574200
H	-3.30055700	1.09106800	-2.31075100
C	-1.48218500	0.08210800	-0.53065000
N	-0.85114600	-1.06374700	-0.72880300
N	-0.82104000	1.22289400	-0.40913000
Si	-1.47548200	-2.65152200	-1.09952800
C	-3.08623400	-2.64944700	-2.09018500
C	-1.74383200	-3.72416500	0.42491200
C	-0.14549700	-3.45268200	-2.17085300
Si	-1.34647900	2.86207300	-0.13925300
C	0.03447200	3.71768000	0.81668400
C	-2.95567800	3.08855400	0.82970600
C	-1.54270700	3.75967900	-1.78973200
H	-2.94642200	2.54988000	1.78827700
H	-3.83814300	2.75526600	0.26499300
H	-3.08336700	4.16034200	1.05086300
H	-0.62794900	3.67722600	-2.39628600
H	-1.74179100	4.83030400	-1.62674800
H	-2.37954400	3.35136000	-2.37647000
H	0.23308800	3.21722200	1.77742700

H	-0.22360800	4.76566900	1.03297400
H	0.97275100	3.71320200	0.24202500
H	-3.95221300	-2.34393200	-1.48308900
H	-3.28014700	-3.66709500	-2.46471300
H	-3.02668200	-1.97691900	-2.96002800
H	-2.55084500	-3.31246500	1.04931000
H	-0.83237400	-3.80076200	1.03585000
H	-2.03193300	-4.74140700	0.11669600
H	-0.01392800	-2.89493100	-3.11269200
H	-0.40239200	-4.49002600	-2.43376400
H	0.82340500	-3.46713200	-1.64774700
Na	0.89581600	0.11759600	-1.78837600
N	2.70675100	-0.01587800	-0.38135400
Na	0.76356200	-0.05458000	0.94482700
Si	3.45500400	-1.47271300	0.11008500
C	2.17634500	-2.51832900	1.06526900
C	4.90063600	-1.24493100	1.31789000
C	4.08525800	-2.52846600	-1.33018200
Si	3.54003200	1.42028600	-0.78567400
C	2.46326200	2.42248700	-2.00957700
C	5.18729600	1.16591800	-1.69018000
C	3.88799500	2.53174900	0.70750400
H	1.97742500	-2.07389600	2.05682000
H	2.53911700	-3.54153600	1.24646300
H	1.21963400	-2.59399000	0.52104100
H	3.27296700	-2.75470100	-2.03918700
H	4.51322500	-3.48328300	-0.98707600
H	4.86772100	-1.98525600	-1.88300900
H	4.56625500	-0.69792400	2.21423800
H	5.72572200	-0.67112600	0.86846100
H	5.30793800	-2.21479900	1.64447000
H	5.03476100	0.59571100	-2.62019100
H	5.91014400	0.60923200	-1.07401900
H	5.64865500	2.13023000	-1.95545100
H	2.40288000	1.91659300	-2.99127700
H	2.89381000	3.41659200	-2.20430600
H	1.44068300	2.58398500	-1.62868600
H	2.96144000	2.74912500	1.26206000
H	4.34828900	3.49031800	0.42149300
H	4.57602100	2.01709000	1.39697800
N	-0.21931300	-0.27077200	3.12217600
C	-1.22569700	0.77702200	3.21865500
H	-1.93922800	0.66994900	2.38957700
H	-0.75446000	1.76886700	3.16122500

H	-1.78838600	0.71519200	4.17341400
C	0.74011700	-0.17901500	4.21084400
H	0.25190200	-0.29808100	5.19993000
H	1.24322000	0.79868200	4.18962800
H	1.50409200	-0.96344500	4.10934900
C	-0.87182300	-1.57434800	3.09595300
H	-1.58001600	-1.60691400	2.25535000
H	-1.42934800	-1.76769600	4.03593200
H	-0.12466000	-2.37017300	2.96590400

Table S71. Atomic coordinates and single point energies for **88**.



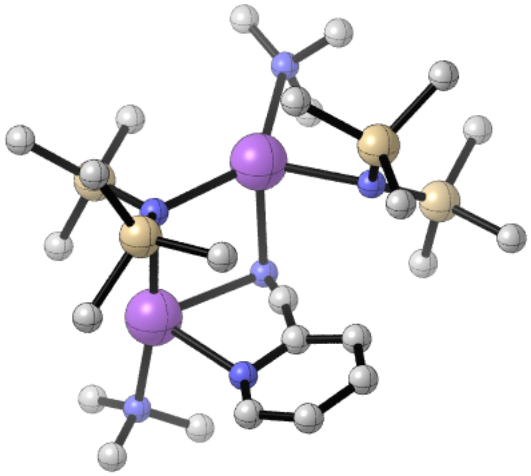
G = –2758.020414
G_{SP} = –2759.987621

N	4.07284600	-1.11203400	0.44533800
C	5.04449000	-0.90915500	1.32677100
C	4.14157200	-0.45904100	-0.71557000
C	6.12929000	-0.06189300	1.08466000
C	5.17920300	0.40864400	-1.06534500
C	6.19668000	0.60450100	-0.13481300
H	4.95733400	-1.44467500	2.27646900
H	6.89960500	0.06990500	1.84432200
H	7.02596100	1.27592700	-0.35968600
H	5.17058400	0.91625700	-2.02902600
C	3.05080100	-0.70712800	-1.64008800
N	2.17830000	-0.92213600	-2.36441900
Na	0.34254500	-1.05743100	-0.31628900
Na	-1.64274100	1.14011500	0.13277400
N	0.70787000	1.28744500	-0.00834500
N	-2.05435800	-1.15481100	0.01852400
Si	0.92529900	2.45058900	-1.24191500
Si	1.29689000	1.49253300	1.58404700
C	-0.16945400	2.03324000	-2.73633400
C	2.67863400	2.64304100	-1.95300700
C	0.47902200	4.21322100	-0.66661200
C	0.24137900	2.68051600	2.63413500
C	3.05964900	2.19242600	1.70709400
C	1.30952800	-0.19530200	2.45312300
Si	-2.88811500	-1.39179900	1.49178600

Si	-2.58381000	-1.74335900	-1.49946000
C	-2.60635200	0.09767100	2.65291400
C	-2.33083800	-2.90034700	2.49854800
C	-4.77485500	-1.56109000	1.33856600
C	-3.88073000	-0.62613300	-2.33073500
C	-3.36457800	-3.47637500	-1.49439800
C	-1.13231300	-1.76375800	-2.72519500
H	0.25645100	1.16634600	-3.26622200
H	-0.21576700	2.87154300	-3.44915700
H	-1.20792000	1.77232400	-2.46848600
H	2.94783900	1.78708100	-2.59018700
H	3.42514900	2.74273900	-1.14941300
H	2.73073000	3.54979900	-2.57680000
H	-0.48473800	4.23624600	-0.13443000
H	0.42410300	4.92156900	-1.50873800
H	1.24037300	4.58966900	0.03637000
H	0.32021500	3.70492400	2.23663500
H	0.57917900	2.70039500	3.68270900
H	-0.82616500	2.40672600	2.64121600
H	3.08841800	3.23511200	1.35102200
H	3.76753100	1.61500300	1.09299200
H	3.42195200	2.18510500	2.74762400
H	0.33241500	-0.70339300	2.37776700
H	1.55496000	-0.11652000	3.52364900
H	2.06489100	-0.84231300	1.97982900
H	-1.53994200	0.24433100	2.88496300
H	-3.12643600	-0.06037200	3.61043500
H	-2.99585000	1.04441400	2.23994700
H	-1.24932700	-2.87077000	2.70640900
H	-2.54855400	-3.83659900	1.96062200
H	-2.85711600	-2.94121200	3.46517700
H	-5.21053900	-0.73914400	0.75001800
H	-5.24849300	-1.55491400	2.33325800
H	-5.05285600	-2.50561600	0.84680500
H	-4.38766800	-3.44152600	-1.09021900
H	-2.79260000	-4.19493200	-0.88871000
H	-3.43113100	-3.87376000	-2.51976300
H	-4.81018300	-0.59847300	-1.73994000
H	-4.13613700	-0.98355000	-3.34086300
H	-3.50442500	0.40639300	-2.43100400
H	-0.72132100	-0.75060100	-2.86049100
H	-1.46986100	-2.10533000	-3.71600300
H	-0.29504900	-2.41732500	-2.43190600
N	-3.39232700	2.84927000	0.05701500

C	-3.29329900	3.50603100	-1.24134000
H	-2.30235900	3.96531700	-1.36400200
H	-3.43672600	2.76967000	-2.04489800
H	-4.06461100	4.29496000	-1.35638900
C	-4.67513300	2.16608100	0.17434900
H	-4.76186800	1.39714000	-0.60566500
H	-4.75545200	1.67421500	1.15371800
H	-5.52258900	2.87427400	0.07039200
C	-3.23378500	3.81936300	1.13260500
H	-3.29076400	3.31539200	2.10814000
H	-2.25547600	4.31411500	1.05931100
H	-4.02343300	4.59766900	1.09691500
N	1.19218500	-3.42163700	-0.00234500
C	1.69319200	-3.57350100	1.35681800
H	2.61630600	-2.99044900	1.47411500
H	0.94920900	-3.20635900	2.07739100
H	1.90700000	-4.63774000	1.59032100
C	2.19669300	-3.87599300	-0.95242600
H	1.85759600	-3.69330800	-1.98199600
H	3.13249100	-3.32368200	-0.78972400
H	2.40442800	-4.96004300	-0.83315400
C	-0.03716500	-4.18747400	-0.16222300
H	-0.82290300	-3.77243500	0.48270500
H	-0.38579100	-4.13182200	-1.20195000
H	0.11636800	-5.25666500	0.09445900

Table S72. Atomic coordinates and single point energies for **69**.



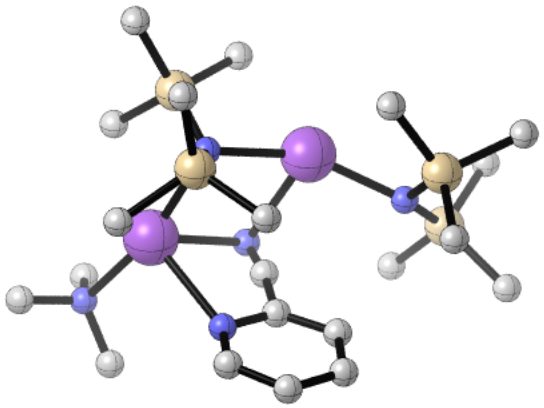
G = –2757.996898
G_{SP} = –2759.966283

N	-1.69362900	-2.44069400	0.07095600
C	-1.93914600	-3.39184200	0.96527200
C	-0.42502700	-2.28019400	-0.33652500
C	-0.94187500	-4.22464100	1.47965400
C	0.64610300	-3.03894500	0.12497900
C	0.36825600	-4.04045100	1.05439900
H	-2.97519300	-3.49288400	1.30082100
H	-1.19765800	-4.98768700	2.21453900
H	1.17986000	-4.65017300	1.45339000
H	1.65610700	-2.80298200	-0.19872600
C	-0.26804800	-1.19532200	-1.29129500
N	-0.35675500	-0.30560400	-2.02364600
Na	-2.69024300	-0.25778700	-0.52994000
Na	0.80251700	1.23623900	-0.06986000
N	-1.50678600	1.22303500	0.87220700
Si	-2.25062600	2.63942800	0.26740600
C	-3.05102000	3.81694600	1.51395300
C	-3.66220300	2.21507400	-0.96734900
C	-1.03085600	3.65411000	-0.75162800
Si	-1.90592100	0.51454800	2.38171900
C	-0.69981700	-0.86282700	2.88240900
C	-3.64516700	-0.30034800	2.29358100
H	-4.40559200	0.43876500	1.98778800
H	-3.95197400	-0.69694900	3.27435800
H	-3.69220800	-1.15031700	1.58808500
H	0.03014700	-0.49832900	3.62103900

H	-0.12225400	-1.23224000	2.02218800
H	-1.23105400	-1.71262800	3.34062100
H	-0.19354400	3.99534900	-0.12353600
H	-1.50469800	4.54298800	-1.19629200
H	-0.61101200	3.05405900	-1.57652500
H	-4.45094700	1.58782600	-0.51214500
H	-3.28538500	1.71078700	-1.87520400
H	-4.15721100	3.13597000	-1.31180500
H	-3.89637100	3.34516700	2.03884700
H	-3.43465200	4.70765700	0.99183400
H	-2.32805700	4.15101300	2.27306900
C	-1.97453400	1.66760700	3.88221300
H	-1.04731500	2.25917900	3.94714200
H	-2.05229600	1.06629100	4.80219500
H	-2.82266000	2.36543800	3.86038300
N	2.53251400	-0.41268000	-0.06912400
Si	3.06839500	-0.23940300	1.54366200
C	2.84739500	-1.78773600	2.62995300
C	2.13479600	1.19817500	2.38647700
C	4.90622000	0.21602100	1.76049700
Si	3.51729300	-1.17310800	-1.23823800
C	2.55365900	-1.72248400	-2.78668400
C	4.36704500	-2.77557400	-0.62694500
C	4.96376400	-0.13542600	-1.91424100
H	1.03798600	1.09933500	2.35180000
H	2.40955300	2.15790000	1.91501000
H	2.41190300	1.27323300	3.44951200
H	5.56937700	-0.56240400	1.35095700
H	5.15079300	0.33097900	2.82869200
H	5.15564800	1.16287200	1.25638600
H	1.79528000	-2.09815900	2.70947600
H	3.22207600	-1.60854100	3.65065400
H	3.42408400	-2.62631500	2.20592800
H	1.80165000	-2.49914100	-2.56843000
H	3.25973800	-2.15151600	-3.51552500
H	2.02731400	-0.88869800	-3.27527700
H	4.62197800	0.72970000	-2.50228000
H	5.59496100	-0.75520800	-2.57102300
H	5.59732500	0.24410000	-1.09756300
H	3.65894100	-3.54550200	-0.27823000
H	5.05284100	-2.56596300	0.20933700
H	4.96204000	-3.22467900	-1.43812700
N	2.26483700	3.04351700	-1.31609100
C	2.05112600	4.45407700	-1.58991000

H	1.08193600	4.60777000	-2.08142600
H	2.05710000	5.02623700	-0.65090500
H	2.84625900	4.86165500	-2.24895400
C	2.16909200	2.27014400	-2.54477100
H	2.31247000	1.20304200	-2.32431900
H	1.17543800	2.40290400	-2.99893600
H	2.93421100	2.57749400	-3.28935200
C	3.56818500	2.85335400	-0.69439900
H	3.62477900	3.43447100	0.23789000
H	3.71197600	1.79008900	-0.46440400
H	4.39019200	3.18945700	-1.36195600
N	-4.06406000	-1.28381100	-2.22693300
C	-3.20507500	-2.14249300	-3.03350900
H	-2.51026800	-1.52918400	-3.62356200
H	-2.61671100	-2.80085800	-2.37887300
H	-3.79673800	-2.77465300	-3.72632600
C	-4.83596400	-0.39240400	-3.08201000
H	-5.45293900	0.28090900	-2.47123800
H	-4.15802900	0.22096800	-3.69143100
H	-5.50140200	-0.95988800	-3.76379600
C	-4.94657000	-2.08249100	-1.38779100
H	-4.34678400	-2.73537700	-0.73677000
H	-5.56343500	-1.42616400	-0.75554500
H	-5.62545800	-2.72097300	-1.98891900

Table S73. Atomic coordinates and single point energies for **90**.



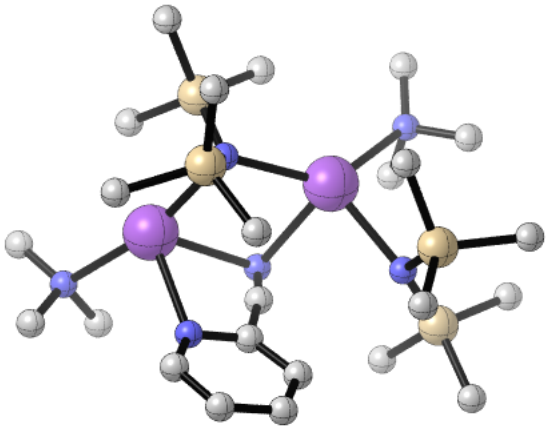
G = –2583.855497
G_{SP} = –2585.62505

N	-1.15322800	-1.81221500	1.51366000
C	-1.08694500	-1.97568600	2.82958200
C	-0.00754300	-1.89914900	0.82054200
C	0.11262600	-2.23211600	3.50116300
C	1.24582400	-2.11741500	1.38656900
C	1.29304400	-2.29299300	2.77030900
H	-2.02656700	-1.88788000	3.38190400
H	0.11147600	-2.35657300	4.58393400
H	2.25167900	-2.45376200	3.26461900
H	2.13818400	-2.08100800	0.76268200
C	-0.19806700	-1.70658400	-0.60622400
N	-0.53305000	-1.50615000	-1.69417600
Na	-2.57209400	-0.49899100	-0.12086600
Na	0.79146500	0.94537000	-0.85087100
N	-1.35545000	1.49552300	-0.08900000
Si	-1.94822700	2.22565700	-1.51413500
C	-2.73254400	3.93585400	-1.35076900
C	-3.26575800	1.10371700	-2.32768400
C	-0.56990400	2.36284900	-2.81970400
Si	-1.62420400	1.90419000	1.54814600
C	-0.22586000	1.28287300	2.67551900
C	-3.23769500	1.06583500	2.17508600
H	-4.08784400	1.33135900	1.52161100
H	-3.49526100	1.40313400	3.19114900
H	-3.16864300	-0.03617400	2.22561700
H	0.50339300	2.08207700	2.87859900
H	0.33128800	0.44889300	2.21856700
H	-0.61536300	0.94236400	3.64857700

H	0.27109300	2.98174100	-2.46229300
H	-0.94691200	2.84215500	-3.73565000
H	-0.18082300	1.37619400	-3.12779800
H	-4.13264700	0.93733900	-1.66178600
H	-2.82844600	0.12790200	-2.60159200
H	-3.66061800	1.54519600	-3.25548300
H	-3.63111900	3.90334600	-0.71500800
H	-3.03344200	4.31447100	-2.34003700
H	-2.03251900	4.65867600	-0.90589700
C	-1.83307300	3.74085100	1.94337800
H	-0.97407900	4.31304900	1.55848000
H	-1.87189100	3.88750600	3.03447200
H	-2.74787200	4.16925900	1.50953100
N	2.78846100	-0.03039200	-0.51613800
Si	3.50096700	1.09636600	0.54615000
C	3.62077900	0.47508900	2.34090200
C	2.45488300	2.69801800	0.58856800
C	5.24091000	1.69948000	0.08242000
Si	3.69120300	-1.15545400	-1.42550600
C	2.59567700	-2.48530900	-2.22806800
C	4.93552600	-2.14039500	-0.36449300
C	4.68662900	-0.39743200	-2.85068500
H	1.39997000	2.55000200	0.87574700
H	2.47761800	3.18879300	-0.40022000
H	2.87227000	3.41623600	1.31145600
H	5.96481900	0.87126700	0.03134700
H	5.61326500	2.42454500	0.82347100
H	5.23038700	2.19397800	-0.90143100
H	2.62083700	0.28143400	2.76095600
H	4.12460900	1.20389700	2.99542800
H	4.19713400	-0.46467000	2.37500900
H	2.06097400	-3.10110400	-1.48532100
H	3.22288000	-3.16779300	-2.82347500
H	1.84119700	-2.04629200	-2.89853900
H	4.01812400	0.15437800	-3.53041500
H	5.20849400	-1.17015700	-3.43714000
H	5.43952500	0.31169600	-2.47531100
H	4.42682300	-2.70649600	0.43430100
H	5.66419900	-1.47369800	0.12338100
H	5.50007900	-2.86497400	-0.97257100
N	-4.04513000	-2.27321800	-0.76926200
C	-5.38797900	-1.95465400	-0.30271200
H	-5.37981100	-1.78224400	0.78357700
H	-5.75088100	-1.04235500	-0.79754400

H	-6.10455400	-2.77296000	-0.51757800
C	-4.03179600	-2.46750500	-2.21521500
H	-4.43849500	-1.57893700	-2.71639000
H	-2.99933200	-2.61918800	-2.56180100
H	-4.63953300	-3.34636100	-2.51066500
C	-3.53544900	-3.46210200	-0.09750000
H	-2.50769100	-3.66687200	-0.43073900
H	-3.51701700	-3.30446300	0.98981300
H	-4.15931000	-4.35189800	-0.31709700

Table S74. Atomic coordinates and single point energies for **89**.



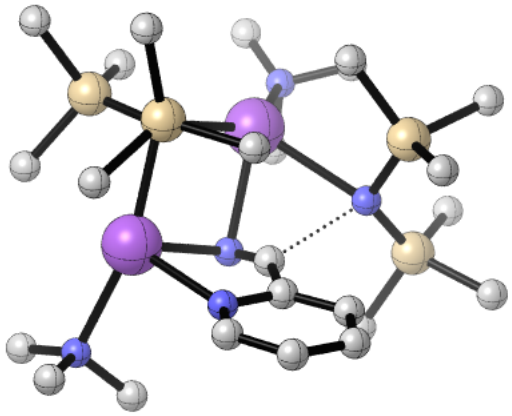
G = –2757.996823
G_{SP} = –2759.966332

N	-1.74700600	-2.41208400	-0.07447000
C	-2.00983500	-3.39103000	0.78481000
C	-0.47158300	-2.24256500	-0.45502200
C	-1.02469400	-4.24465800	1.28756900
C	0.58876200	-3.02201100	-0.00224500
C	0.29250200	-4.05301700	0.88827200
H	-3.05186800	-3.49931800	1.09913000
H	-1.29534500	-5.02975000	1.99329800
H	1.09564400	-4.67901300	1.27918200
H	1.60490900	-2.77539400	-0.29779700
C	-0.29078200	-1.12526000	-1.36708400
N	-0.34463300	-0.20723300	-2.06699300
Na	-2.74517200	-0.19887500	-0.51586500
Na	0.87778000	1.20802300	-0.05486200
N	-1.45555500	1.21821700	0.86055200
Si	-2.11607400	2.67574100	0.25850300
C	-2.98206100	3.82206100	1.49114400
C	-3.43874600	2.33617000	-1.09347400
C	-0.80857800	3.70435900	-0.62927500
Si	-1.90293000	0.49793400	2.34891100
C	-0.75600300	-0.93104000	2.84305500
C	-3.66242400	-0.27349500	2.20912700
H	-4.39274600	0.46892300	1.84199100
H	-4.02057900	-0.62287500	3.19026400
H	-3.69949500	-1.15296000	1.53983100
H	-0.00822300	-0.60389100	3.58132400
H	-0.19877900	-1.32193500	1.97877600

H	-1.32433400	-1.75876400	3.29758000
H	0.01163300	3.97390800	0.05396700
H	-1.23165700	4.63679400	-1.03423200
H	-0.37374600	3.14594600	-1.47505100
H	-4.30934200	1.77710700	-0.70650800
H	-3.01820100	1.79020100	-1.95840800
H	-3.83019500	3.28582700	-1.48931800
H	-3.85143400	3.33655800	1.96179200
H	-3.34096100	4.72558000	0.97348700
H	-2.29863600	4.13810400	2.29343600
C	-1.97201000	1.62653400	3.86695800
H	-1.03291000	2.19568000	3.95652300
H	-2.08071600	1.01464000	4.77667200
H	-2.80349600	2.34412900	3.83886900
N	2.56660900	-0.47233100	-0.09009300
Si	3.07844600	-0.37721900	1.53638800
C	2.78528600	-1.95560500	2.56089200
C	2.17055100	1.05368100	2.41755400
C	4.92614800	0.00571300	1.80154400
Si	3.53800400	-1.22247300	-1.27667900
C	2.56871600	-1.67257200	-2.85258500
C	4.31785400	-2.87762300	-0.71554300
C	5.03156500	-0.21600600	-1.89438900
H	1.07222000	0.97995300	2.36522100
H	2.47215900	2.02302100	1.98369500
H	2.43452500	1.08502100	3.48610000
H	5.56767700	-0.78294500	1.37711900
H	5.15515000	0.07554600	2.87704800
H	5.21906900	0.95871400	1.33408000
H	1.72020700	-2.22290300	2.62278200
H	3.15936500	-1.83087000	3.58986000
H	3.32892100	-2.80174700	2.10899900
H	1.78749000	-2.42898100	-2.66894600
H	3.26243400	-2.09715000	-3.59574900
H	2.07604200	-0.80054300	-3.30865400
H	4.73187300	0.68581000	-2.44927400
H	5.64527800	-0.83330800	-2.56981400
H	5.67020500	0.10364400	-1.05628200
H	3.57484900	-3.63103300	-0.40538300
H	4.99819400	-2.72450800	0.13741900
H	4.90749500	-3.31999900	-1.53426100
N	2.44540300	3.03315500	-1.19023900
C	2.28415500	4.46172600	-1.39756600
H	1.32739100	4.67335400	-1.89182900

H	2.29755800	4.98714200	-0.43169500
H	3.10131200	4.87287800	-2.02688800
C	2.33847700	2.32245200	-2.45489700
H	2.44060300	1.24174300	-2.28323300
H	1.35671500	2.51263500	-2.91475800
H	3.12391000	2.63568400	-3.17560100
C	3.73271000	2.76768900	-0.56377400
H	3.79758500	3.30117900	0.39605800
H	3.83564400	1.69043400	-0.38366400
H	4.57489300	3.10606600	-1.20471400
N	-4.39476600	-1.11531900	-2.01560500
C	-3.53412700	-1.57064300	-3.10105100
H	-3.03983700	-0.71144300	-3.57731900
H	-2.75661600	-2.23980600	-2.70417000
H	-4.10524000	-2.12071800	-3.87606200
C	-5.42490600	-0.21713900	-2.51874500
H	-6.04604700	0.14534700	-1.68748000
H	-4.96427900	0.65178500	-3.00750200
H	-6.08421200	-0.72609500	-3.25083000
C	-4.99984700	-2.24910600	-1.33068500
H	-4.21197500	-2.91473900	-0.95233300
H	-5.60392700	-1.89703700	-0.48183000
H	-5.65623700	-2.83454200	-2.00622900

Table S75. Atomic coordinates and single point energies for **TS-19**.



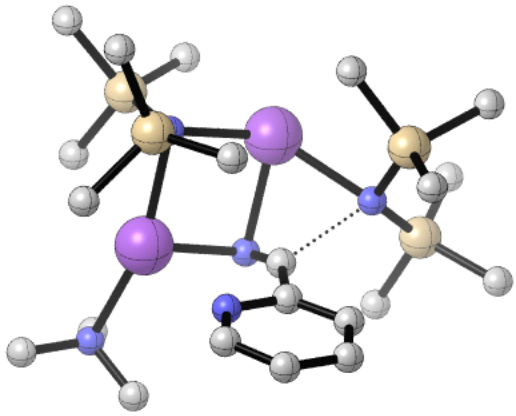
G = –2757.98648
G_{SP} = –2759.952416

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.32929733
C	1.18252269	0.00000000	-0.63741814
C	1.16906681	-0.03344815	2.09060250
C	2.40213244	-0.02882108	0.03142272
C	2.38879725	-0.05851204	1.42394230
H	-0.97801115	0.03705763	1.81861536
H	1.11318774	-0.03193513	3.17889018
H	3.32872029	-0.07782890	1.97736582
H	3.32410497	0.00692026	-0.53977109
C	1.03503957	0.03082790	-2.10327807
N	0.32334925	-0.18825670	-3.00928248
Na	-1.66359807	0.42741993	-1.75378902
Na	0.71911092	2.15020445	-3.69207793
N	-1.25620753	2.69893666	-2.34727630
Si	-2.53636250	2.82613157	-3.47062255
C	-3.67210592	4.33498454	-3.34877084
C	-3.70992620	1.30981001	-3.37013632
C	-1.86698868	2.76651455	-5.23839673
Si	-1.28971545	3.41607357	-0.79161302
C	0.37409231	3.28171243	0.12004361
C	-2.59070615	2.55428398	0.32308869
H	-3.59610957	2.64129816	-0.12224344
H	-2.63299080	3.01147102	1.32453973
H	-2.38185387	1.47963265	0.47426170
H	0.94364769	4.22088695	0.04261332
H	1.00812364	2.48432124	-0.29176082

H	0.22067410	3.07875104	1.19251221
H	-1.16464105	3.59483912	-5.42308664
H	-2.67102113	2.83111832	-5.98780611
H	-1.32975574	1.81920873	-5.41451940
H	-4.11369282	1.15858603	-2.35247025
H	-3.20504457	0.38156482	-3.69102814
H	-4.57486470	1.43757810	-4.03931127
H	-4.23653683	4.34203395	-2.40318887
H	-4.40089565	4.32465771	-4.17450695
H	-3.10156001	5.27404822	-3.40652805
C	-1.71740968	5.26114395	-0.71979286
H	-1.07244615	5.82513313	-1.41262683
H	-1.53400153	5.64513709	0.29659053
H	-2.76320060	5.47590429	-0.97960314
N	2.90652385	1.08277401	-2.77008480
Si	3.56424394	2.59758194	-2.26571543
C	4.02083188	2.73049666	-0.42529997
C	2.36746630	4.03343205	-2.64625596
C	5.16483086	3.10392125	-3.16450161
Si	3.96367448	-0.19737834	-3.25249540
C	3.07100690	-1.86726245	-3.35502611
C	5.41601495	-0.50073420	-2.04695678
C	4.81416936	0.01614403	-4.93938375
H	1.35922303	3.91998223	-2.21852264
H	2.27414456	4.19158599	-3.73482733
H	2.77916055	4.96631759	-2.23087675
H	5.97862438	2.37830209	-3.01382716
H	5.50829830	4.07343983	-2.76957097
H	5.01800890	3.22109066	-4.24864624
H	3.15685138	2.63588668	0.24737785
H	4.48338895	3.71271529	-0.23783819
H	4.76034827	1.96002524	-0.15125373
H	2.65586108	-2.17322575	-2.38092875
H	3.78877260	-2.64072930	-3.67056407
H	2.23917212	-1.85065472	-4.07468076
H	4.10002275	-0.00002313	-5.77551112
H	5.51662514	-0.81928570	-5.08882389
H	5.38918868	0.95187740	-5.00205361
H	5.09727663	-0.91844246	-1.07872342
H	5.98775934	0.41766980	-1.84191710
H	6.11279910	-1.22951609	-2.49057893
N	1.41224262	2.14449825	-6.13189015
C	0.76509632	2.73822773	-7.29046993
H	-0.27092766	2.38635985	-7.37300485

H	0.75098174	3.83332106	-7.19380835
H	1.30041735	2.47830524	-8.22725308
C	1.35918804	0.69025535	-6.20563050
H	1.81862759	0.25239277	-5.30748426
H	0.31305593	0.35358518	-6.25243465
H	1.89117675	0.30437824	-7.10071618
C	2.79347092	2.59687315	-6.04952854
H	2.82590797	3.69484900	-5.99180740
H	3.26512815	2.17503500	-5.15292079
H	3.38160248	2.27938283	-6.93647628
N	-2.62878149	-1.78094405	-1.52938873
C	-1.49049920	-2.68956458	-1.59087224
H	-1.03786775	-2.65399001	-2.59095445
H	-0.72782258	-2.38076658	-0.86244048
H	-1.79170572	-3.73352185	-1.36731859
C	-3.63786242	-2.16317177	-2.50542991
H	-4.47799338	-1.45538112	-2.48098730
H	-3.20378932	-2.14883868	-3.51505409
H	-4.02947986	-3.18250555	-2.30917733
C	-3.19303910	-1.74831542	-0.18916470
H	-2.41927505	-1.44162375	0.52982025
H	-4.02046080	-1.02437267	-0.14428372
H	-3.58206289	-2.73920671	0.12377654

Table S76. Atomic coordinates and single point energies for **TS-20**.



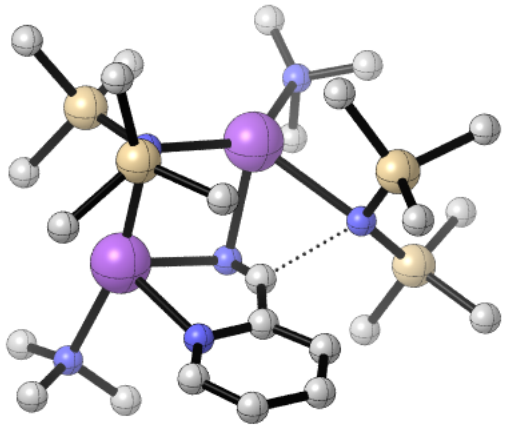
G = –2583.842873
G_{SP} = –2585.608845

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.32986753
C	1.18252246	0.00000000	-0.63328456
C	1.17030135	-0.03184668	2.08876914
C	2.40600991	-0.02657652	0.03082192
C	2.39216369	-0.05666229	1.42276595
H	-0.97863113	0.03028478	1.81826049
H	1.11594972	-0.03218426	3.17716769
H	3.33024189	-0.07762588	1.97918326
H	3.32597761	0.00585917	-0.54842307
C	1.03752453	0.00401044	-2.09716826
N	0.33696181	-0.29227894	-2.99267632
Na	-1.71095506	0.26251932	-1.82530949
Na	0.66430750	2.11366682	-3.49512863
N	-1.41390487	2.52700443	-2.47400347
Si	-2.34937853	2.59378066	-3.89683618
C	-3.63226385	3.97380680	-4.03895314
C	-3.28058605	0.94901034	-4.16715840
C	-1.21441840	2.73958207	-5.42671260
Si	-1.74527035	3.20692222	-0.94252777
C	-0.19371517	3.36070671	0.14540857
C	-2.96210713	2.08609643	0.03465785
H	-3.86291521	1.87503507	-0.56771385
H	-3.29753141	2.57335150	0.96353541
H	-2.51431121	1.12181408	0.33537412
H	0.28907358	4.34183602	0.01652008
H	0.55569040	2.58984332	-0.09191743

H	-0.45635251	3.26183863	1.21129369
H	-0.55250351	3.62035369	-5.36067702
H	-1.81166658	2.86116499	-6.34290036
H	-0.59909557	1.83610300	-5.58898959
H	-3.95074779	0.71946435	-3.31932671
H	-2.55968831	0.12161152	-4.28299009
H	-3.90146179	0.96348324	-5.07619671
H	-4.42416549	3.85692916	-3.28277576
H	-4.10981229	3.95299553	-5.03098415
H	-3.17676394	4.96516621	-3.89663948
C	-2.53701677	4.92617109	-0.93692743
H	-1.93861853	5.62365144	-1.54416298
H	-2.57327995	5.32082940	0.09098666
H	-3.56151349	4.92421651	-1.33591031
N	2.73883588	1.25189252	-2.72436772
Si	3.31350540	2.78643064	-2.16721968
C	3.73135308	2.88345967	-0.31981605
C	2.03067903	4.16125887	-2.50600111
C	4.84430898	3.44095185	-3.08097380
Si	3.83116870	0.13972266	-3.48127511
C	3.09990092	-1.59320284	-3.69949538
C	5.40916312	-0.15771293	-2.45273581
C	4.37329158	0.68247485	-5.21298424
H	1.02330052	3.98868537	-2.09590397
H	1.94332774	4.35606280	-3.59063848
H	2.39109984	5.09992507	-2.05740588
H	5.71073755	2.76545453	-3.03620575
H	5.14535028	4.40260258	-2.63563999
H	4.61435501	3.62281303	-4.14188313
H	2.85396834	2.71898178	0.32274163
H	4.13230505	3.88307002	-0.08910396
H	4.50247507	2.14468458	-0.04743233
H	2.80249912	-2.04153510	-2.73792979
H	3.86901910	-2.24234536	-4.14743261
H	2.21641728	-1.59441233	-4.35327427
H	3.48852497	0.85825651	-5.84582188
H	4.98063814	-0.10024133	-5.69411983
H	4.96617846	1.60770152	-5.19604053
H	5.18960979	-0.75375160	-1.55147078
H	5.89432692	0.77409182	-2.12578235
H	6.14577965	-0.72884306	-3.03985675
N	-2.61518088	-1.96653532	-1.78009814
C	-1.65078307	-2.67015303	-0.94527537
H	-0.63992895	-2.54045626	-1.35905658

H	-1.66053043	-2.25744741	0.07321432
H	-1.87575812	-3.75490365	-0.88942710
C	-2.58250028	-2.49842149	-3.13694420
H	-3.32965730	-1.98620602	-3.75805428
H	-1.58789950	-2.33092632	-3.57532064
H	-2.80165149	-3.58566589	-3.15135282
C	-3.95362599	-2.05535459	-1.21707987
H	-3.96777898	-1.62039467	-0.20715843
H	-4.66228098	-1.49668041	-1.84504146
H	-4.30480680	-3.10536480	-1.14787753

Table S77. Atomic coordinates and single point energies for **TS-21**.



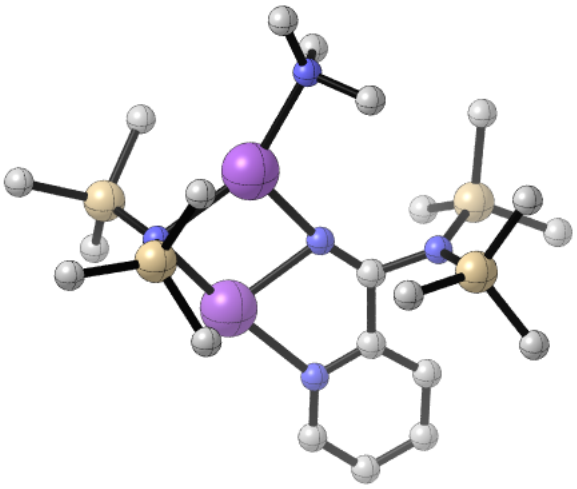
G = –2757.98648
G_{SP} = –2759.952416

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.32929733
C	1.18252269	0.00000000	-0.63741814
C	1.16906681	-0.03344815	2.09060250
C	2.40213244	-0.02882108	0.03142272
C	2.38879725	-0.05851204	1.42394230
H	-0.97801115	0.03705763	1.81861536
H	1.11318774	-0.03193513	3.17889018
H	3.32872029	-0.07782890	1.97736582
H	3.32410497	0.00692026	-0.53977109
C	1.03503957	0.03082790	-2.10327807
N	0.32334925	-0.18825670	-3.00928248
Na	-1.66359807	0.42741993	-1.75378902
Na	0.71911092	2.15020445	-3.69207793
N	-1.25620753	2.69893666	-2.34727630
Si	-2.53636250	2.82613157	-3.47062255
C	-3.67210592	4.33498454	-3.34877084
C	-3.70992620	1.30981001	-3.37013632
C	-1.86698868	2.76651455	-5.23839673
Si	-1.28971545	3.41607357	-0.79161302
C	0.37409231	3.28171243	0.12004361
C	-2.59070615	2.55428398	0.32308869
H	-3.59610957	2.64129816	-0.12224344
H	-2.63299080	3.01147102	1.32453973
H	-2.38185387	1.47963265	0.47426170
H	0.94364769	4.22088695	0.04261332
H	1.00812364	2.48432124	-0.29176082

H	0.22067410	3.07875104	1.19251221
H	-1.16464105	3.59483912	-5.42308664
H	-2.67102113	2.83111832	-5.98780611
H	-1.32975574	1.81920873	-5.41451940
H	-4.11369282	1.15858603	-2.35247025
H	-3.20504457	0.38156482	-3.69102814
H	-4.57486470	1.43757810	-4.03931127
H	-4.23653683	4.34203395	-2.40318887
H	-4.40089565	4.32465771	-4.17450695
H	-3.10156001	5.27404822	-3.40652805
C	-1.71740968	5.26114395	-0.71979286
H	-1.07244615	5.82513313	-1.41262683
H	-1.53400153	5.64513709	0.29659053
H	-2.76320060	5.47590429	-0.97960314
N	2.90652385	1.08277401	-2.77008480
Si	3.56424394	2.59758194	-2.26571543
C	4.02083188	2.73049666	-0.42529997
C	2.36746630	4.03343205	-2.64625596
C	5.16483086	3.10392125	-3.16450161
Si	3.96367448	-0.19737834	-3.25249540
C	3.07100690	-1.86726245	-3.35502611
C	5.41601495	-0.50073420	-2.04695678
C	4.81416936	0.01614403	-4.93938375
H	1.35922303	3.91998223	-2.21852264
H	2.27414456	4.19158599	-3.73482733
H	2.77916055	4.96631759	-2.23087675
H	5.97862438	2.37830209	-3.01382716
H	5.50829830	4.07343983	-2.76957097
H	5.01800890	3.22109066	-4.24864624
H	3.15685138	2.63588668	0.24737785
H	4.48338895	3.71271529	-0.23783819
H	4.76034827	1.96002524	-0.15125373
H	2.65586108	-2.17322575	-2.38092875
H	3.78877260	-2.64072930	-3.67056407
H	2.23917212	-1.85065472	-4.07468076
H	4.10002275	-0.00002313	-5.77551112
H	5.51662514	-0.81928570	-5.08882389
H	5.38918868	0.95187740	-5.00205361
H	5.09727663	-0.91844246	-1.07872342
H	5.98775934	0.41766980	-1.84191710
H	6.11279910	-1.22951609	-2.49057893
N	1.41224262	2.14449825	-6.13189015
C	0.76509632	2.73822773	-7.29046993
H	-0.27092766	2.38635985	-7.37300485

H	0.75098174	3.83332106	-7.19380835
H	1.30041735	2.47830524	-8.22725308
C	1.35918804	0.69025535	-6.20563050
H	1.81862759	0.25239277	-5.30748426
H	0.31305593	0.35358518	-6.25243465
H	1.89117675	0.30437824	-7.10071618
C	2.79347092	2.59687315	-6.04952854
H	2.82590797	3.69484900	-5.99180740
H	3.26512815	2.17503500	-5.15292079
H	3.38160248	2.27938283	-6.93647628
N	-2.62878149	-1.78094405	-1.52938873
C	-1.49049920	-2.68956458	-1.59087224
H	-1.03786775	-2.65399001	-2.59095445
H	-0.72782258	-2.38076658	-0.86244048
H	-1.79170572	-3.73352185	-1.36731859
C	-3.63786242	-2.16317177	-2.50542991
H	-4.47799338	-1.45538112	-2.48098730
H	-3.20378932	-2.14883868	-3.51505409
H	-4.02947986	-3.18250555	-2.30917733
C	-3.19303910	-1.74831542	-0.18916470
H	-2.41927505	-1.44162375	0.52982025
H	-4.02046080	-1.02437267	-0.14428372
H	-3.58206289	-2.73920671	0.12377654

Table S78. Atomic coordinates and single point energies for **70**.



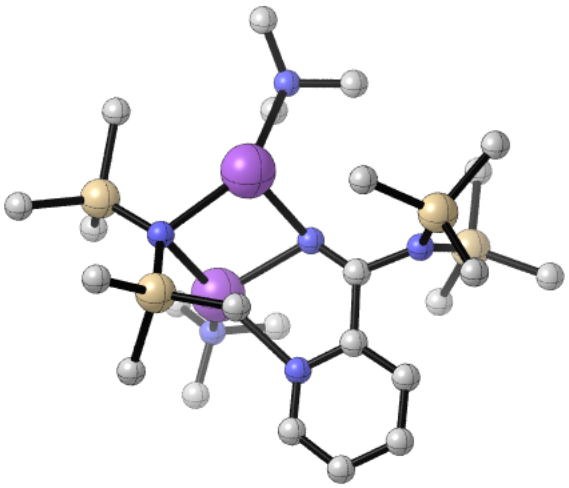
G = –2583.883064
G_{SP} = –2585.643535

N	0.84726100	2.95020700	0.39062800
C	1.13431200	4.24843000	0.45749000
C	1.84411700	2.04743300	0.40701200
C	2.43122400	4.74576400	0.56473600
C	3.17909600	2.46785100	0.50468500
C	3.47382900	3.82516600	0.59436600
H	0.28550300	4.93895200	0.42579100
H	2.60824600	5.81939500	0.62242700
H	4.50945200	4.15890800	0.68137800
H	3.97137400	1.72196300	0.50338100
C	1.45468600	0.56095700	0.35058500
N	0.30305900	0.14794200	0.57820800
Na	-1.25212200	1.88078700	0.45865000
Na	-1.55662600	-1.08187000	0.22165600
N	-3.13895200	0.64374700	0.01203400
Si	-4.11613100	0.37678300	1.37515400
C	-5.97811400	0.26360700	1.06764400
C	-3.82698900	1.72218200	2.68346200
C	-3.60748500	-1.26334100	2.22050500
Si	-3.41298400	0.67022500	-1.66530900
C	-3.02027500	-1.03081100	-2.44250100
C	-2.19969500	1.89019800	-2.47420500
H	-2.37381700	2.91908500	-2.11577700
H	-2.29720300	1.90619900	-3.57068300
H	-1.15345200	1.61605900	-2.25178300
H	-3.60947300	-1.82132600	-1.94710300

H	-1.94978200	-1.28837200	-2.34428800
H	-3.25172300	-1.06418700	-3.51840300
H	-3.70058600	-2.11191000	1.51880800
H	-4.23669200	-1.49448200	3.09360000
H	-2.56574900	-1.22105100	2.58696000
H	-4.10331900	2.71195500	2.28588800
H	-2.76600400	1.75788900	2.98639700
H	-4.41609800	1.55110700	3.59765300
H	-6.35784700	1.17886600	0.58868900
H	-6.52501500	0.11996700	2.01255700
H	-6.21717800	-0.58386600	0.40599400
C	-5.15369100	1.14203700	-2.23172700
H	-5.89913900	0.40019600	-1.90838300
H	-5.20071900	1.21479900	-3.32955300
H	-5.44814100	2.11685800	-1.81281500
N	2.61636500	-0.28032700	0.00286500
Si	3.04121700	-0.37603200	-1.69965900
C	4.46478000	0.77178600	-2.17483900
C	1.52546800	0.12139600	-2.69434100
C	3.57163600	-2.13030600	-2.14472500
Si	3.44877500	-1.11780400	1.30218600
C	2.87327900	-0.38656400	2.93401900
C	5.31387900	-0.86969100	1.11211100
C	3.16003000	-2.98161000	1.33869000
H	1.27121500	1.17521200	-2.50013200
H	0.65435000	-0.48732500	-2.40855800
H	1.70204300	0.00665800	-3.77434900
H	4.47165100	-2.44082800	-1.59214700
H	3.81017500	-2.18185600	-3.21827400
H	2.77571200	-2.86024900	-1.93616900
H	4.17395800	1.82891900	-2.08382700
H	4.76439100	0.59249000	-3.21943400
H	5.34719100	0.60386500	-1.53823900
H	3.06394100	0.69673100	2.97572000
H	3.39658600	-0.86203700	3.77719100
H	1.79112100	-0.53941400	3.05824300
H	2.11403600	-3.22265000	1.57147600
H	3.79216100	-3.43504500	2.11861700
H	3.41426300	-3.45616000	0.37972100
H	5.59198100	0.19497300	1.14720600
H	5.68498700	-1.28273000	0.16109600
H	5.85099100	-1.38242500	1.92502900
N	-0.95005200	-3.35556900	0.02105100
C	-1.81564200	-4.39443500	-0.50929100

H	-2.74357800	-4.44672700	0.07825500
H	-2.07846200	-4.16412700	-1.55128200
H	-1.32976600	-5.39145900	-0.48258100
C	-0.62935500	-3.59049900	1.42104700
H	-0.04445400	-2.74269200	1.81228100
H	-1.55448400	-3.67887400	2.00882600
H	-0.03455200	-4.51679900	1.56150000
C	0.26532600	-3.21248000	-0.77128500
H	0.00162000	-3.02853900	-1.82404400
H	0.85417900	-2.35585600	-0.40134100
H	0.89378000	-4.12697900	-0.72621200

Table S79. Atomic coordinates and single point energies for **87**.



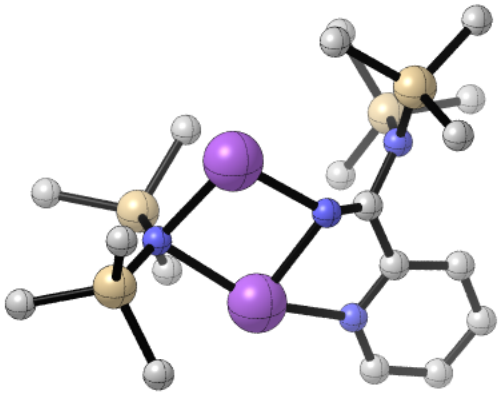
G = –2758.027861
G_{SP} = –2759.987108

N	0.21646300	-2.51114400	0.01800700
C	0.08663400	-3.80140800	0.31629400
C	1.39851800	-1.90270600	0.22616400
C	1.11873000	-4.58595600	0.82851100
C	2.49201700	-2.62451600	0.72786500
C	2.35161600	-3.97584500	1.03135400
H	-0.90022300	-4.24576600	0.14797800
H	0.95010400	-5.63759900	1.05875200
H	3.19633900	-4.54220100	1.42768700
H	3.43732000	-2.11030100	0.88624800
C	1.46671900	-0.39478500	-0.05913800
N	0.49334400	0.27571700	-0.44477000
Na	-1.49518000	-0.90997600	-0.73713400
Na	-0.90455900	1.75494900	0.57163800
N	-2.75942800	0.38162800	0.87626900
Si	-4.05754100	1.14605700	0.07987600
C	-5.77792900	0.96001300	0.84737100
C	-4.19295600	0.51456900	-1.71139800
C	-3.72360100	3.01280900	-0.06489600
Si	-2.87047100	-0.84023600	2.06503900
C	-1.19862200	-1.11256100	2.91514800
C	-3.36853000	-2.51338900	1.28326100
H	-4.36847100	-2.43191500	0.82576200
H	-3.40304500	-3.32640800	2.02577100
H	-2.66925100	-2.83170700	0.49011400
H	-0.98698300	-0.28831200	3.61520100

H	-0.37911200	-1.16359700	2.18132300
H	-1.19385100	-2.04955400	3.49432700
H	-3.61644800	3.46837100	0.93312000
H	-4.52920600	3.54297700	-0.59590600
H	-2.79180100	3.20030900	-0.62371600
H	-4.35236500	-0.57784100	-1.71661500
H	-3.25810700	0.71980800	-2.26056600
H	-5.01654600	0.97809300	-2.27680400
H	-6.08032500	-0.09768600	0.90517600
H	-6.52696500	1.49111500	0.23912600
H	-5.80896400	1.37456000	1.86628000
C	-4.11250200	-0.54456600	3.46549600
H	-3.96378400	0.45262300	3.90895700
H	-3.97342900	-1.29331300	4.26157100
H	-5.15450300	-0.60843800	3.12056900
N	2.81218300	0.15716500	0.23638200
Si	3.07134900	0.89209300	1.80715800
C	3.75170100	-0.35092500	3.05364300
C	1.45269500	1.56417700	2.50526500
C	4.28384300	2.33295600	1.68748300
Si	3.99310200	0.13792800	-1.06280900
C	3.41322500	-1.05019300	-2.40103100
C	5.66595400	-0.45546000	-0.41546100
C	4.20969200	1.82402700	-1.87799800
H	0.67650400	0.78627900	2.52002100
H	1.10804600	2.42671800	1.91576300
H	1.60638200	1.90612300	3.54035100
H	5.25918500	2.04554300	1.26892100
H	4.46291600	2.73679700	2.69610500
H	3.87436000	3.14388800	1.06698400
H	3.02648500	-1.15874700	3.23707600
H	3.96572600	0.13760300	4.01690600
H	4.68626000	-0.80672600	2.69012600
H	3.27752100	-2.07455700	-2.02327600
H	4.15149100	-1.07878600	-3.21709100
H	2.45512300	-0.70681200	-2.81708900
H	3.26180100	2.13995300	-2.34038300
H	4.97349100	1.77063800	-2.66963700
H	4.51558300	2.60055000	-1.16212500
H	5.59489800	-1.49171200	-0.04970100
H	6.05062400	0.16488800	0.40731300
H	6.41506000	-0.43772800	-1.22222700
N	-0.03685100	3.67852000	-0.73522300
C	-0.56724400	5.03029300	-0.64716600

H	-1.64569000	5.03154900	-0.85720100
H	-0.41297400	5.42946700	0.36542600
H	-0.07046400	5.71182200	-1.36822100
C	-0.26971400	3.11275300	-2.05961300
H	0.13721300	2.09128100	-2.08385700
H	-1.34912600	3.07656200	-2.27322700
H	0.21636300	3.72137800	-2.85036400
C	1.39295300	3.66911100	-0.44978900
H	1.58131700	4.13203200	0.53043100
H	1.75606600	2.62878200	-0.43887800
H	1.96198700	4.24344600	-1.21105100
N	-1.55096300	-1.75946500	-3.05204100
C	-0.12551200	-1.62850400	-3.31984100
H	0.14051300	-0.56391000	-3.38863900
H	0.45340300	-2.06450400	-2.49424500
H	0.16411900	-2.13163000	-4.26608400
C	-2.32693800	-1.16199700	-4.12570400
H	-3.40017000	-1.22362400	-3.90143900
H	-2.06074900	-0.10123000	-4.23529700
H	-2.13718000	-1.66946400	-5.09457800
C	-1.91940400	-3.15401800	-2.86887600
H	-1.32358100	-3.59044100	-2.05482000
H	-2.98483700	-3.23079700	-2.60611700
H	-1.74236700	-3.75456900	-3.78550700

Table S80. Atomic coordinates and single point energies for **93**.

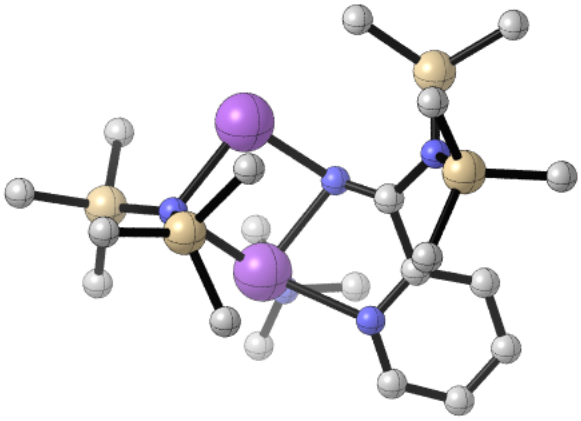


G = –2409.727928
G_{SP} = –2411.290157

N	-0.57665800	2.63075200	0.56115200
C	-0.81574300	3.94173600	0.54555600
C	-1.60575900	1.78281400	0.71466100
C	-2.08403600	4.49358900	0.71189600
C	-2.91311000	2.25224300	0.90060200
C	-3.15275100	3.62196800	0.90970400
H	0.04977500	4.59409400	0.39367200
H	-2.22066400	5.57452500	0.69349600
H	-4.16251600	4.00673100	1.06456000
H	-3.71499300	1.52706300	1.03606000
C	-1.28456000	0.29118700	0.73347100
N	-0.21905100	-0.15894000	1.20707000
Na	1.44959800	1.36735700	0.80189200
Na	1.28474600	-1.71323800	0.69970600
N	2.89591100	-0.27531900	-0.08599100
Si	2.57454300	-0.15540200	-1.75200600
C	3.97012300	-0.67113800	-2.91732200
C	2.06354300	1.61134500	-2.24729800
C	1.06741300	-1.25620500	-2.14871100
Si	4.28586200	-0.20330200	0.88695000
C	4.34063500	-1.70310000	2.05448000
C	4.19958800	1.32345500	2.03147500
H	4.12600700	2.25435300	1.44234800
H	5.09102100	1.41765300	2.67051500
H	3.33228600	1.26731600	2.71366300
H	4.38968900	-2.64063800	1.47651800
H	3.43940900	-1.73613400	2.69231200
H	5.20830000	-1.68430700	2.73171200

H	1.30256900	-2.32838300	-2.01920700
H	0.72213300	-1.13018900	-3.18685200
H	0.21578400	-0.99773600	-1.49232200
H	2.88235100	2.31741500	-2.02972300
H	1.16305000	1.95842900	-1.70960700
H	1.83612700	1.68774300	-3.32220100
H	4.84041300	-0.00515100	-2.81732800
H	3.63813600	-0.64040600	-3.96683800
H	4.30597600	-1.69604200	-2.69530600
C	5.94230200	-0.11488900	-0.01869100
H	6.07761300	-0.98286100	-0.68186400
H	6.78267700	-0.09345000	0.69245600
H	6.00180900	0.79261800	-0.64004600
N	-2.38723400	-0.52127900	0.23955900
Si	-2.58015700	-2.01392300	1.16049100
C	-2.50138200	-1.65806100	3.00146600
C	-1.29479300	-3.34491400	0.71185600
C	-4.29874900	-2.71332100	0.81010000
Si	-2.99171600	-0.31849300	-1.41042700
C	-2.05051800	1.06352100	-2.27870000
C	-4.83286000	0.08136400	-1.44203600
C	-2.70308000	-1.89697000	-2.40714800
H	-0.50638000	-3.38310400	1.48156800
H	-0.84686900	-3.13301400	-0.27247800
H	-1.74165300	-4.34944700	0.66114000
H	-5.07128200	-1.99963100	1.13491000
H	-4.43511500	-3.63925300	1.39052500
H	-4.48267700	-2.95508400	-0.24625200
H	-1.51505300	-1.26756600	3.28464900
H	-2.70355100	-2.57468700	3.57706700
H	-3.26043000	-0.91003500	3.27740500
H	-2.34920400	2.06399200	-1.93376100
H	-2.25213500	1.00282800	-3.35978400
H	-0.96364400	0.96198000	-2.13462400
H	-1.62501600	-2.06838400	-2.54621800
H	-3.15860200	-1.79502800	-3.40464900
H	-3.13109100	-2.79371200	-1.93656700
H	-5.03820100	1.04422800	-0.95089300
H	-5.42624900	-0.69483100	-0.93777300
H	-5.18539700	0.15425600	-2.48267500

Table S81. Atomic coordinates and single point energies for **92**.



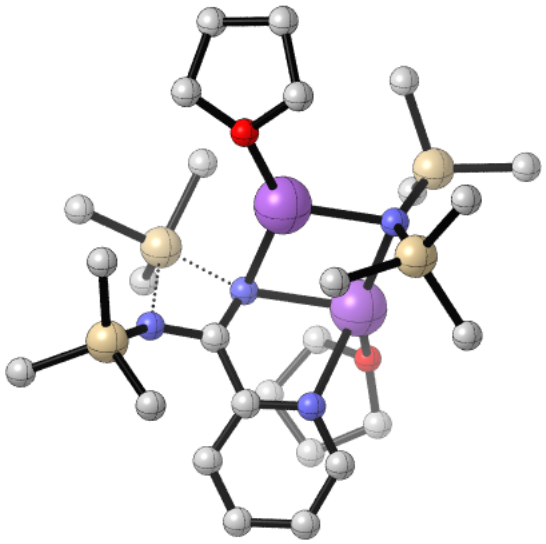
G = –2583.879458
G_{SP} = –2585.640023

N	0.56352000	1.89641300	-1.46259700
C	0.69674700	2.90874100	-2.31794500
C	1.60951800	1.54410200	-0.70321300
C	1.86396500	3.66035100	-2.44167000
C	2.82182600	2.24589200	-0.75850700
C	2.94413600	3.32584300	-1.62624100
H	-0.17578100	3.14029700	-2.93773100
H	1.91686700	4.48392900	-3.15341100
H	3.87347300	3.89664600	-1.67374000
H	3.64210700	1.92789200	-0.11459300
C	1.40002200	0.39959000	0.28143200
N	0.33057400	0.25265900	0.91296800
Na	-1.44591700	1.08639200	-0.35118200
Na	-1.02387100	-1.44713300	1.36569100
N	-2.61672900	-1.01620700	-0.22998100
Si	-4.13596800	-0.79285400	0.49356900
C	-5.46807300	-2.07911400	0.10368800
C	-4.88653000	0.89885600	0.05310600
C	-3.90874100	-0.84248700	2.38883600
Si	-2.06020700	-1.84022800	-1.61276000
C	-0.45182300	-2.76458000	-1.15855500
C	-1.59710400	-0.64752700	-3.01740900
H	-2.48409400	-0.07223300	-3.33132000
H	-1.21785200	-1.18545900	-3.90057100
H	-0.81502400	0.06820900	-2.71212600
H	-0.64676400	-3.57589300	-0.43363200
H	0.28745300	-2.06803400	-0.72206700

H	0.02421100	-3.22902600	-2.03652900
H	-3.62177300	-1.86125200	2.70520000
H	-4.82849100	-0.58715800	2.93741400
H	-3.12606200	-0.14200900	2.72689600
H	-5.16491100	0.90923000	-1.01316100
H	-4.16169100	1.71546200	0.20771700
H	-5.78752100	1.13549600	0.64043600
H	-5.72938300	-2.07830300	-0.96513200
H	-6.38604400	-1.87146400	0.67608000
H	-5.12805700	-3.09350700	0.36382400
C	-3.23765200	-3.11878000	-2.35917300
H	-3.56449100	-3.85333200	-1.60755800
H	-2.74599200	-3.66416500	-3.18008100
H	-4.13799400	-2.63593200	-2.76937900
N	2.59858300	-0.40004800	0.47095800
Si	3.40431500	-1.18367800	-0.89648900
C	5.20844000	-0.65864400	-1.03707900
C	2.52149300	-0.76269500	-2.50696800
C	3.33214100	-3.06027300	-0.69530100
Si	2.75733000	-0.95771000	2.13818500
C	2.44134400	0.45465900	3.33635300
C	4.54258200	-1.50842600	2.41511600
C	1.61394000	-2.42260600	2.54946500
H	2.75373300	0.25120000	-2.86402700
H	1.42831200	-0.84558700	-2.40620900
H	2.84426800	-1.47723200	-3.28057900
H	3.73765900	-3.41163600	0.26434800
H	3.90993700	-3.54408000	-1.49839600
H	2.29141700	-3.40958900	-0.77252600
H	5.29031100	0.42266900	-1.22376400
H	5.69012100	-1.18153600	-1.87798400
H	5.77417300	-0.89313600	-0.12406700
H	3.06725600	1.32147200	3.07267800
H	2.69901500	0.15090800	4.36288200
H	1.38959900	0.76865400	3.30821100
H	0.74726700	-2.07494500	3.13528300
H	2.12342900	-3.18946700	3.15242200
H	1.26747100	-2.90870600	1.62294400
H	5.22794100	-0.65892300	2.27244700
H	4.87232700	-2.32441600	1.75661600
H	4.65385100	-1.85571900	3.45431400
N	-1.68430600	3.18367200	0.95854500
C	-2.12512900	2.59449100	2.21477200
H	-3.14775100	2.20205400	2.11450600

H	-1.44854200	1.76782700	2.48006400
H	-2.11802800	3.33547500	3.04139600
C	-2.57517600	4.25325500	0.54159800
H	-2.24384500	4.66034800	-0.42454600
H	-3.60012800	3.87315800	0.42533500
H	-2.59599500	5.08378100	1.27779400
C	-0.31961200	3.67487700	1.10226900
H	0.33775700	2.83918100	1.38095200
H	0.03507200	4.09735200	0.15106800
H	-0.25709900	4.46365600	1.88091300

Table S82. Atomic coordinates and single point energies for **TS-9**.



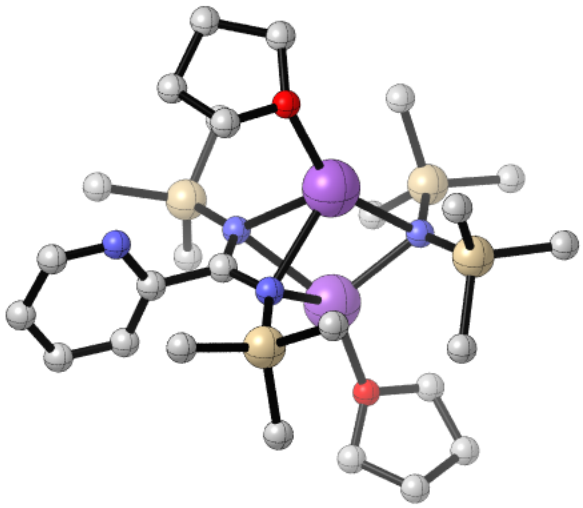
G = –2873.868031
G_{SP} = –2875.95519

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.33270948
C	1.17607780	0.00000000	-0.64131980
C	1.16348927	0.04308608	2.09976913
C	2.39450394	0.07116460	0.04472064
C	2.38657421	0.09952456	1.43522180
H	-0.97925972	-0.03296322	1.82046401
H	1.10315555	0.04376465	3.18789608
H	3.32214614	0.15846778	1.99389113
H	3.32075743	0.10360442	-0.52945824
C	1.16321816	0.01240707	-2.14870233
N	0.25124365	0.62945662	-2.82728482
Na	-1.69023709	0.96525526	-1.50333295
Na	-1.31283724	-0.80565741	-3.84281815
N	2.20500127	-0.46335236	-2.88335628
N	-3.18685888	-0.50620963	-2.55815980
Si	1.40053158	0.60249244	-4.40531150
Si	2.98551507	-2.02792790	-2.76937501
C	2.17442305	2.31777193	-4.19402725
C	-0.11509483	0.82435566	-5.62410514
C	2.50370899	-0.26799849	-5.72766033
C	4.84304474	-1.86094461	-3.01196856
C	2.27409912	-3.20640292	-4.06653502
C	2.67127845	-2.87723212	-1.10826576

Si	-4.34702682	0.47545247	-3.32705557
Si	-3.31725424	-1.88178632	-1.56159254
C	-4.61270074	-0.02099306	-5.14439023
C	-3.70447549	2.26713445	-3.35590313
C	-6.05567180	0.51170406	-2.51249213
C	-4.73744771	-3.07173642	-1.96687602
C	-3.52396405	-1.42383765	0.27042723
C	-1.68568997	-2.85692469	-1.68675328
H	1.41041944	3.07850986	-3.97682962
H	2.70898005	2.61762303	-5.10755526
H	2.89986139	2.30654805	-3.36666291
H	-0.93466056	1.41566619	-5.18064413
H	-0.53555415	-0.12781584	-6.00056406
H	0.22884885	1.35560947	-6.52534894
H	3.52193448	-0.47112918	-5.36061616
H	2.58324265	0.39452543	-6.60511012
H	2.08133706	-1.21891064	-6.08733186
H	5.08303818	-1.39211139	-3.97698266
H	5.33020262	-2.84765968	-2.98226755
H	5.28370598	-1.23892456	-2.21791898
H	2.66365352	-3.00319298	-5.07317961
H	1.17406825	-3.12415222	-4.09732389
H	2.52502035	-4.24709670	-3.80898806
H	3.23049621	-2.43313778	-0.27345933
H	2.98843814	-3.92809006	-1.20015026
H	1.60221693	-2.87668037	-0.84169943
H	-3.65039192	-0.07936073	-5.68418695
H	-5.25128585	0.69696660	-5.68225715
H	-5.09604024	-1.01023089	-5.20425284
H	-2.70455646	2.31850176	-3.82118700
H	-3.62615926	2.68816738	-2.33875354
H	-4.36437320	2.93339562	-3.93241531
H	-6.53513795	-0.47847087	-2.55084159
H	-6.72442881	1.22814297	-3.01470995
H	-5.97565227	0.80629667	-1.45426290
H	-4.45812178	-0.85973832	0.42057870
H	-2.68630258	-0.78614158	0.59764256
H	-3.54752032	-2.30725351	0.92736949
H	-5.71069781	-2.58909493	-1.78835027
H	-4.68984514	-3.97070058	-1.33221577
H	-4.71538564	-3.40017181	-3.01739900
H	-1.51681597	-3.25947222	-2.70012734
H	-1.65393076	-3.70727440	-0.98825919
H	-0.83939496	-2.19374818	-1.43192064

O	-1.35737182	-2.55390027	-5.23047935
C	-2.66424014	-3.12113628	-5.30772826
C	-0.68516610	-2.89576163	-6.43290545
C	-3.04876722	-3.09161137	-6.80108795
C	-1.74218851	-2.68010332	-7.51187979
H	-1.77024517	-1.61624395	-7.78780184
H	-1.54285267	-3.26192949	-8.42049386
H	0.20175696	-2.25540118	-6.52456047
H	-0.35851587	-3.95036577	-6.38631457
H	-3.39728242	-4.07883985	-7.13107497
H	-3.85379241	-2.37125193	-6.99343670
H	-2.63363954	-4.15296096	-4.91819592
H	-3.32383292	-2.52150821	-4.66371316
O	-1.29322127	3.03951713	-0.72183350
C	-0.85172649	3.41068488	0.57206265
H	-1.21269091	2.65956326	1.28762999
H	-1.29030436	4.38837783	0.83958528
C	0.67982685	3.49833795	0.47245122
H	1.14968346	2.58062888	0.85116190
H	1.06886581	4.33950509	1.06090484
C	0.93685670	3.65891838	-1.04350143
H	1.44235561	2.77277984	-1.44920652
H	1.54452352	4.53963031	-1.28792851
C	-0.46956321	3.74834253	-1.64060161
H	-0.55547260	3.26443403	-2.62278824
H	-0.82153081	4.79307392	-1.71107752

Table S83. Atomic coordinates and single point energies for **71**.



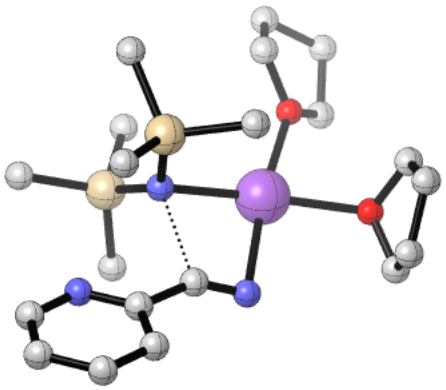
G = –2873.907517
G_{SP} = –2875.996392

N	3.86905100	-0.72617900	-0.31701500
C	5.05788400	-1.30841300	-0.17258800
C	2.82400300	-1.27161800	0.30425800
C	5.26571100	-2.45620200	0.59104600
C	2.92471600	-2.42316000	1.09530600
C	4.16980600	-3.02483400	1.23925800
H	5.89640500	-0.83667000	-0.69416000
H	6.26229700	-2.88973300	0.67317000
H	4.28696700	-3.92314500	1.84789400
H	2.03543700	-2.82623600	1.58402500
C	1.48477100	-0.58892700	0.12973600
N	0.69340200	-0.96348600	-0.86439600
Na	-0.11847200	1.37378400	-0.88927300
Na	-1.11754200	-0.64578500	0.77683500
N	1.13623100	0.35915900	0.98374300
N	-2.36556900	1.04333700	-0.19463300
Si	0.89260600	-2.24721300	-2.03027700
Si	1.94442500	0.94164900	2.41850700
C	0.04617300	-3.80205400	-1.36210400
C	2.66753900	-2.71378200	-2.48477800
C	0.05349600	-1.72412400	-3.62962900
C	1.26358600	0.02104600	3.92125900
C	1.55924700	2.78019100	2.55068800
C	3.82654600	0.75996100	2.50470400
Si	-3.11474200	0.61341100	-1.65872000

Si	-2.67074100	2.26640700	0.94507000
C	-3.22033900	-1.28118400	-1.79680100
C	-2.10614800	1.23507100	-3.15199600
C	-4.87504400	1.25971300	-1.92832200
C	-4.46352500	2.85575300	1.10017200
C	-1.60580700	3.80824100	0.59482900
C	-2.15495200	1.64915800	2.66750500
H	0.54428300	-4.14435400	-0.44066800
H	0.08541400	-4.62562000	-2.09159200
H	-1.01347800	-3.60750900	-1.13230700
H	3.21482900	-3.19244900	-1.65870700
H	3.24216700	-1.83033100	-2.80147300
H	2.63793200	-3.42266400	-3.32761100
H	-1.00817000	-1.48343500	-3.47929000
H	0.12090200	-2.52885400	-4.37799600
H	0.54704400	-0.83304300	-4.04904600
H	0.16773300	0.08762500	3.98882500
H	1.68475700	0.42457400	4.85507000
H	1.53874300	-1.04432700	3.86384800
H	0.48022200	2.96390200	2.65554800
H	1.90376400	3.30285200	1.64297900
H	2.06926600	3.23177400	3.41520300
H	4.14557200	-0.29224900	2.55611900
H	4.17272200	1.26067400	3.42329100
H	4.33972200	1.22461500	1.65071000
H	-2.25351100	-1.74428300	-1.53791800
H	-3.49475700	-1.62069100	-2.80814700
H	-3.97980300	-1.66564300	-1.09723700
H	-1.07792400	0.83690400	-3.16943700
H	-2.04318700	2.33610100	-3.12558100
H	-2.56633700	0.95009100	-4.11125000
H	-5.53549200	0.98801300	-1.09014000
H	-5.30323600	0.83754800	-2.85131500
H	-4.88929100	2.35653100	-2.02269500
H	-1.81982500	4.19752700	-0.41456800
H	-0.53232300	3.55514000	0.64361700
H	-1.77380400	4.62263600	1.31696900
H	-4.82083900	3.33355300	0.17607100
H	-4.55859100	3.58608400	1.91924800
H	-5.13556800	2.01119300	1.32077200
H	-2.78626500	0.80455400	2.98979800
H	-2.22520900	2.43194000	3.43895400
H	-1.10853100	1.30446400	2.64534800
O	-2.49745900	-2.16016600	1.67838700

C	-3.85796300	-1.72367600	1.76289300
C	-2.47927000	-3.57891600	1.68514100
C	-4.72090700	-2.90579400	1.27271700
C	-3.68926800	-3.96119800	0.84428300
H	-3.44188100	-3.85095800	-0.22170500
H	-4.02586500	-4.99096400	1.01927200
H	-1.51837600	-3.91286600	1.27137200
H	-2.57325700	-3.95392600	2.72078600
H	-5.34931200	-3.28636000	2.08951600
H	-5.38724400	-2.61846600	0.44908400
H	-4.09070800	-1.46181100	2.80765800
H	-3.94612200	-0.81741800	1.14416400
O	1.44147300	2.62273800	-1.89004400
C	1.77613900	3.98427700	-1.63014000
H	1.06085200	4.37026100	-0.89044500
H	1.66397300	4.57182300	-2.55555800
C	3.23828000	3.98454500	-1.13138900
H	3.34263900	4.46854400	-0.15163000
H	3.88321100	4.52555100	-1.83764500
C	3.60352600	2.49340900	-1.09053800
H	3.36720300	2.04746200	-0.11440000
H	4.65899000	2.28985800	-1.31110700
C	2.65118900	1.90446400	-2.11700100
H	2.45983500	0.83264100	-1.97335700
H	3.00026700	2.07994000	-3.15129400

Table S84. Atomic coordinates and single point energies for **TS-14**.

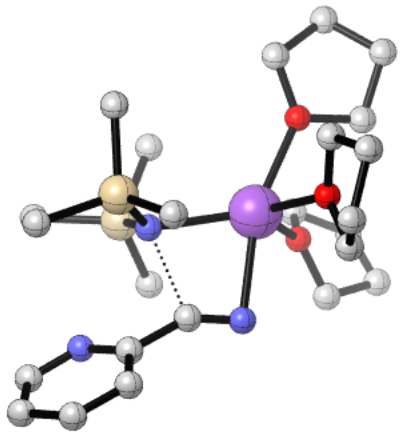


G = –1839.020386
G_{SP} = –1840.520422

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.32786671
C	1.16813262	0.00000000	-0.62796067
C	1.16440283	0.01415115	2.09735708
C	2.39738095	-0.02421222	0.04558909
C	2.38943296	-0.00331646	1.43590960
H	-0.98217867	-0.00472658	1.81126803
H	1.10499114	0.03386068	3.18559598
H	3.32680805	-0.00150373	1.99433630
H	3.32321280	-0.04765980	-0.52865114
C	1.24340925	-0.01373381	-2.10259237
N	1.88369306	-0.36235611	-3.02558634
Na	0.56871181	0.69361745	-4.63886364
N	-0.46092245	1.24228831	-2.63457359
Si	-1.97961507	0.45721444	-2.47898422
Si	-0.06057424	2.87698646	-2.34598686
C	-3.03239858	0.91184800	-0.97172723
C	-1.73662913	-1.41928664	-2.52565210
C	-3.09629399	0.84300293	-3.98004317
C	0.59539314	3.23923861	-0.60392743
C	-1.47444042	4.11989537	-2.59934062
C	1.33756228	3.34958974	-3.55877988
H	-3.36867867	1.91114734	-4.00856241
H	-4.03141909	0.26127961	-3.94444444
H	-2.57921070	0.59643644	-4.92324504
H	-2.49981637	0.68105018	-0.03968010
H	-3.98259282	0.35448893	-0.98002675
H	-3.27757723	1.98548687	-0.97216790

H	-1.14723751	-1.75758118	-1.66103671
H	-1.19937461	-1.72412583	-3.43945268
H	-2.70303234	-1.94699899	-2.51505205
H	2.16936474	2.62969891	-3.46145760
H	1.74424889	4.35484121	-3.36927719
H	0.98427856	3.33297724	-4.60572924
H	-2.27712240	3.94464634	-1.86630160
H	-1.92404862	4.06350274	-3.60159926
H	-1.11009539	5.14927715	-2.45290727
H	-0.13984729	2.91233281	0.14852477
H	0.76870250	4.31847946	-0.46792322
H	1.54152224	2.71647418	-0.39535424
O	-0.53989396	1.55212593	-6.39873612
C	-1.32397156	2.74322492	-6.32569951
C	-0.79838748	0.84433428	-7.61217622
C	-2.41577756	2.56108292	-7.37069320
C	-1.66753782	1.77781852	-8.45139436
H	-1.03762059	2.45733048	-9.04539743
H	-2.32719063	1.23336752	-9.13880550
H	0.16237318	0.58444345	-8.07977182
H	-1.33214992	-0.09036814	-7.37119156
H	-0.68631301	3.61516460	-6.55874942
H	-1.69765992	2.84071106	-5.29801648
H	-3.23458381	1.95649700	-6.95186730
H	-2.83050062	3.51366103	-7.72369441
H	1.76670382	2.39849972	-6.82984042
C	2.61527500	1.70177609	-6.85843312
O	2.21203577	0.50087503	-6.21813998
H	3.62451684	3.02531809	-5.43285637
C	3.86482847	2.18302937	-6.09423840
H	2.85920075	1.48533224	-7.91436311
H	3.16149460	-0.95213424	-5.13107408
C	3.41202149	-0.17098397	-5.85681884
H	4.04996721	1.06244152	-4.21827289
C	4.29194272	0.93838475	-5.28353050
H	4.64673067	2.51499184	-6.78987882
H	3.86309036	-0.62130665	-6.76033385
H	5.36280980	0.71415631	-5.36938536

Table S85. Atomic coordinates and single point energies for **TS-13**.



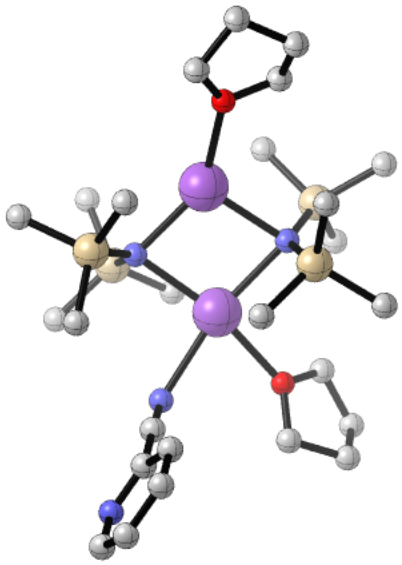
G = –2071.092467
G_{SP} = –2072.855558

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.32633265
C	1.17179927	0.00000000	-0.62971121
C	1.16498182	0.01862830	2.09774975
C	2.39839984	-0.01906159	0.04523597
C	2.38920855	0.00512069	1.43734134
H	-0.98173617	-0.00450907	1.81023503
H	1.10454164	0.04163776	3.18583341
H	3.32647906	0.01222012	1.99604565
H	3.32658307	-0.04467444	-0.52568591
C	1.21826663	-0.00913768	-2.10407935
N	1.70544977	-0.46671297	-3.07157991
Na	0.71844224	1.11815914	-4.58222298
N	-0.06294518	1.67918300	-2.44929343
Si	-1.73427264	1.28784758	-2.45071918
Si	0.66420125	3.10786895	-1.86079516
C	-2.72725033	1.89485905	-0.95550608
C	-1.98379575	-0.58006432	-2.61920958
C	-2.57948507	2.07179634	-3.97283003
C	2.53167203	3.02489829	-2.21460950
C	0.50166069	3.40632710	0.00599324
C	0.00034913	4.66438894	-2.72620049
H	-2.55549018	3.17142303	-3.89783218
H	-3.63146142	1.76019542	-4.07715846
H	-2.04573899	1.78825036	-4.89535601
H	-2.30282067	1.49019965	-0.02510349
H	-3.77921079	1.57567713	-1.02645356

H	-2.71414751	2.99493854	-0.89116248
H	-1.67463364	-1.08437744	-1.69273736
H	-1.35803216	-0.96582404	-3.43871241
H	-3.03632195	-0.83145303	-2.82695583
H	0.08949477	4.56463771	-3.82070755
H	0.54001955	5.57375151	-2.41755563
H	-1.06698006	4.81136328	-2.49491869
H	1.02340462	2.62256840	0.57890415
H	-0.55285597	3.40574607	0.32115384
H	0.94245076	4.37638204	0.28684141
H	3.02512947	2.31109959	-1.53562411
H	3.02225855	4.00354657	-2.09252523
H	2.70403050	2.66869080	-3.24153048
O	0.03801073	2.22913314	-6.50397197
C	-0.53463402	3.51247113	-6.74022585
C	0.48384073	1.64123750	-7.72679730
C	-0.88019460	3.51958729	-8.22342398
C	0.28486548	2.71287045	-8.79900335
H	1.17832408	3.35108340	-8.88260726
H	0.08139466	2.28464379	-9.78882055
H	1.52842026	1.31883213	-7.60204877
H	-0.12479146	0.74578116	-7.93369598
H	0.20594512	4.29805819	-6.50421349
H	-1.39782894	3.63483404	-6.07282201
H	-1.83254432	2.99384645	-8.39243659
H	-0.96566349	4.53175889	-8.63880592
H	2.62193608	3.74212405	-5.19281721
C	3.03302312	3.02878274	-5.92834414
O	2.76576838	1.70054008	-5.48584978
H	4.91372795	4.16036844	-5.86198275
C	4.55419497	3.13663793	-6.02647180
H	2.52513178	3.19731258	-6.89014412
H	3.77346820	0.47622805	-4.17797870
C	3.97348787	1.03736098	-5.10069780
H	4.93481677	2.60274659	-3.95576933
C	5.00944268	2.14595890	-4.95357898
H	4.89721718	2.80724847	-7.01908430
H	4.25988994	0.32448215	-5.89351997
H	6.03671411	1.78707290	-5.09720505
C	0.15802759	-1.90430976	-5.63448053
O	-0.33691636	-0.57534915	-5.66698289
C	-1.62848217	-0.62891047	-6.24952727
C	-1.57581848	-1.77225530	-7.28774193
C	-0.22500192	-2.46236966	-7.00347642

H	1.23344353	-1.86395003	-5.42533718
H	-0.33401291	-2.46438958	-4.81802558
H	-2.37548570	-0.83211786	-5.46320624
H	-1.84113834	0.36061940	-6.67746340
H	-2.42053481	-2.45974251	-7.14984775
H	-1.62687973	-1.39400143	-8.31752720
H	-0.29081229	-3.55771128	-7.01033968
H	0.52697260	-2.16279540	-7.74743009

Table S86. Atomic coordinates and single point energies for **72**.



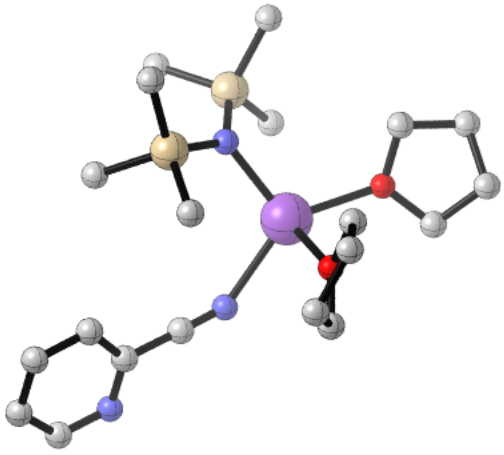
G = –2873.868207
G_{SP} = –2875.965991

N	-5.96667100	-0.87692000	-0.43066700
C	-6.84524100	-1.14062100	-1.39016800
C	-4.72317500	-0.58297000	-0.80616700
C	-6.52548700	-1.11897100	-2.75117400
C	-4.28812000	-0.52809000	-2.13448100
C	-5.22329700	-0.80518800	-3.12789400
H	-7.86037200	-1.38306100	-1.06433600
H	-7.28935400	-1.34571000	-3.49510800
H	-4.93476900	-0.77844700	-4.17926200
H	-3.24996100	-0.27999300	-2.36176000
C	-3.76652500	-0.29894400	0.24869500
N	-2.96814000	-0.05934100	1.04561700
Na	-0.56575500	0.53905700	0.82846400
Na	2.04511100	-0.92675500	0.19731800
N	0.11072600	-1.71555500	1.22087300
N	1.49110500	1.36957200	-0.06986300
Si	-0.29364400	-3.06392600	0.25974100
Si	-0.08561600	-1.65616100	2.91997500
C	0.83526400	-3.09815400	-1.27994500
C	-2.07179600	-3.07463000	-0.40389900
C	-0.00638600	-4.75532300	1.07394200
C	1.33596400	-2.48301300	3.86435200
C	-1.70260500	-2.40428100	3.56702000
C	-0.12205300	0.16915300	3.48812600

Si	2.73624700	2.09545400	0.84034700
Si	0.95978700	1.63963400	-1.66248400
C	3.66278400	0.74080100	1.82245800
C	2.22821100	3.32355200	2.19881900
C	4.00977400	3.09030700	-0.16671500
C	2.16641700	1.00599000	-2.99070900
C	0.53667000	3.43115300	-2.12017600
C	-0.66311200	0.66757900	-1.96878500
H	0.85862500	-2.14377300	-1.83546600
H	0.51917500	-3.87748500	-1.99061000
H	1.86448300	-3.34488500	-0.97313200
H	-2.23811000	-2.20685400	-1.06233900
H	-2.79934200	-3.02132900	0.42124800
H	-2.27600700	-3.98537100	-0.98869500
H	1.04567200	-4.85623000	1.38476500
H	-0.23438100	-5.57653400	0.37599300
H	-0.63145100	-4.89468600	1.96906500
H	1.37356000	-3.55725300	3.62462600
H	1.22206500	-2.38266000	4.95512700
H	2.30697400	-2.04523800	3.58155700
H	-1.77299800	-3.48175700	3.35313600
H	-2.56091200	-1.90708700	3.08906600
H	-1.79389300	-2.27374200	4.65702900
H	0.70803800	0.75400500	3.05546600
H	-0.02682700	0.23564600	4.58238500
H	-1.07766700	0.65730100	3.22602300
H	2.96340700	0.22441500	2.50336300
H	4.45110200	1.17971400	2.45280300
H	4.15137400	-0.02210100	1.19465100
H	1.50389200	2.89730500	2.90933200
H	1.80122200	4.24849400	1.78255200
H	3.12583800	3.60565200	2.77240900
H	4.44568700	2.54398600	-1.01581600
H	4.83749900	3.42572800	0.47824600
H	3.52796800	3.99336600	-0.57510300
H	1.36612600	4.11747500	-1.88940400
H	-0.34639900	3.75830600	-1.54928900
H	0.30370100	3.52932300	-3.19217200
H	3.09971800	1.59255500	-2.98729700
H	1.73187900	1.07377200	-4.00051200
H	2.42779700	-0.04925100	-2.80000700
H	-0.60100900	-0.38156700	-1.63045200
H	-0.91067300	0.65723800	-3.04198300
H	-1.49667000	1.15733100	-1.43858100

O	3.89968900	-1.50366300	-1.07009600
C	4.20219300	-2.61756000	-1.91833600
C	4.82361800	-0.43727100	-1.30817400
C	5.52433800	-2.27493800	-2.59926000
C	5.45572400	-0.74909400	-2.65572000
H	4.79018700	-0.42076200	-3.46843400
H	6.43262500	-0.26664000	-2.78628000
H	4.26505700	0.50701100	-1.28162700
H	5.58431900	-0.42278800	-0.50837800
H	6.37332800	-2.59380100	-1.97633300
H	5.62232200	-2.75080700	-3.58318200
H	4.25024700	-3.53105100	-1.30852100
H	3.38914900	-2.73296700	-2.65285500
O	-1.66327900	2.57188600	0.60768200
C	-2.94654400	2.98574400	0.15692200
C	-0.97882500	3.65372000	1.24482300
C	-2.87446600	4.50647000	0.09384300
C	-1.97810100	4.80893400	1.29548000
H	-3.71885400	2.65025300	0.87054000
H	-3.14684200	2.51356400	-0.81763600
H	-3.86253600	4.98098400	0.15083300
H	-2.38811600	4.82670100	-0.83997700
H	-2.56675300	4.76857900	2.22400100
H	-1.48754700	5.78911100	1.24359900
H	-0.64385100	3.32954200	2.24059100
H	-0.08723800	3.89492800	0.64676800

Table S87. Atomic coordinates and single point energies for **73**.

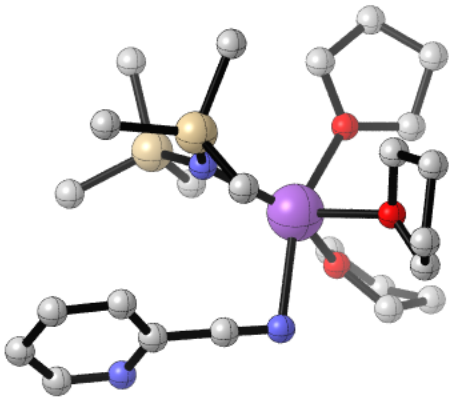


G = –1839.029923
G_{SP} = –1840.535752

N	-4.80660200	-1.12204500	-2.01585400
C	-6.09664800	-0.99246700	-1.73425600
C	-3.93742300	-0.67792200	-1.10814200
C	-6.56928800	-0.42129200	-0.54791900
C	-4.28965000	-0.09496500	0.11230700
C	-5.64853300	0.03397100	0.38990100
H	-6.79728700	-1.35952600	-2.48910400
H	-7.64200300	-0.33812200	-0.37231400
H	-5.97686400	0.48785400	1.32556400
H	-3.51751300	0.24960700	0.80017000
C	-2.52852400	-0.82440600	-1.43295100
N	-1.40173300	-0.92970000	-1.65296900
Na	0.83389900	-0.37584900	-0.87848800
N	0.69793600	1.54072600	0.26838200
Si	1.61043300	2.74863000	-0.49463100
Si	-0.55572100	1.75094300	1.37852300
C	0.70014700	4.38931400	-0.80668200
C	2.13362400	2.15836900	-2.23493200
C	3.18050200	3.24082800	0.46110200
C	-1.14004200	0.05656000	2.04193100
C	-2.10456500	2.59605200	0.64936200
C	-0.11079100	2.76334200	2.92333900
H	2.88683300	3.75569300	1.39013100
H	3.82584500	3.92444200	-0.11351600
H	3.77630900	2.36432400	0.75728400
H	-0.20162600	4.22809200	-1.41813000
H	1.34550800	5.11074200	-1.33313300

H	0.38412600	4.85495500	0.14111800
H	1.23377000	2.07832300	-2.86833200
H	2.63064200	1.17408200	-2.23872100
H	2.81501200	2.87246000	-2.72379700
H	0.75456700	2.31714700	3.43834000
H	-0.94530600	2.82472000	3.64025700
H	0.16742500	3.79221200	2.64308200
H	-2.40367800	2.12419900	-0.30137700
H	-1.87949800	3.65000600	0.42360800
H	-2.96632100	2.58315300	1.33834400
H	-1.33656100	-0.65176600	1.21883400
H	-2.04824000	0.13811300	2.66258300
H	-0.35394200	-0.38647800	2.67511600
O	3.01602100	-1.03870000	-1.05164500
C	4.09153800	-0.34894000	-0.41279100
C	3.41892300	-2.34495500	-1.45832500
C	5.34348600	-1.12719600	-0.79813800
C	4.80628800	-2.55756900	-0.85471100
H	4.72573000	-2.97155600	0.16221900
H	5.42519800	-3.23995500	-1.45121600
H	2.66764600	-3.06769600	-1.10525400
H	3.45219300	-2.38240400	-2.55983300
H	3.92971200	-0.35254800	0.67941100
H	4.09122800	0.69449000	-0.75317500
H	5.69567200	-0.81139500	-1.79158700
H	6.16396700	-0.99216800	-0.08217700
H	1.64182300	-1.04551700	1.67398600
C	1.59343100	-2.12602100	1.46411800
O	0.74069700	-2.30305300	0.33500300
H	0.84634800	-2.35975800	3.52371000
C	0.98061900	-2.95478900	2.61118400
H	2.61021300	-2.47522500	1.21365700
H	-0.98174000	-3.31485600	-0.08515900
C	-0.08547900	-3.43518200	0.53788500
H	-1.16035000	-2.73830900	2.27520200
C	-0.35631000	-3.44754600	2.03752400
H	1.63223100	-3.80380700	2.86076200
H	0.44470400	-4.35347600	0.22059900
H	-0.64341800	-4.43969600	2.40912100

Table S88. Atomic coordinates and single point energies for **74**.



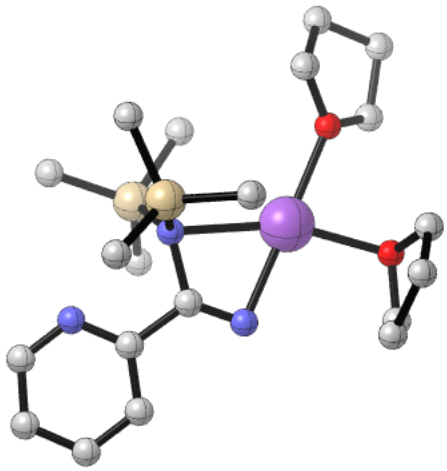
G = –2071.105061
G_{SP} = –2072.873364

N	-3.39606000	-2.88597100	0.67304800
C	-4.66907800	-2.91531100	0.29593700
C	-2.92279000	-1.72590000	1.12730900
C	-5.51453500	-1.80419500	0.36479600
C	-3.66783700	-0.54927500	1.23082200
C	-5.00293000	-0.60160500	0.84156200
H	-5.04124000	-3.87139800	-0.08187000
H	-6.55187600	-1.88714800	0.04025100
H	-5.62818500	0.29051900	0.89865600
H	-3.19842100	0.36370000	1.59406900
C	-1.53289500	-1.72105900	1.54890400
N	-0.43737500	-1.71748600	1.91307100
Na	0.70801200	-0.36865100	0.12052600
N	-1.08518400	0.90508000	-0.55404300
Si	-1.51197600	0.33651900	-2.09395300
Si	-1.58854400	2.35768100	0.14830900
C	-3.28322200	-0.34037600	-2.25508300
C	-0.39380300	-1.14241300	-2.53400500
C	-1.36847300	1.61733600	-3.49811700
C	-1.43376100	2.25674000	2.05952400
C	-3.39728700	2.84465600	-0.21087300
C	-0.59736500	3.89711600	-0.38491200
H	-2.11816800	2.41294100	-3.35435000
H	-1.55195200	1.16511000	-4.48591900
H	-0.38188100	2.10499800	-3.52057900
H	-3.41967300	-1.24126900	-1.63549000
H	-3.50822700	-0.61418400	-3.29865500
H	-4.02491900	0.40824900	-1.93307000

H	-0.54883900	-1.95031700	-1.79658000
H	0.67588200	-0.87458300	-2.51921600
H	-0.62647700	-1.55611900	-3.52750100
H	0.46458400	3.83501800	-0.09676200
H	-1.00959100	4.81525500	0.06445100
H	-0.63666900	4.00858200	-1.48043600
H	-4.10148800	2.05551800	0.09687500
H	-3.54743700	3.00930600	-1.29029900
H	-3.67625700	3.77363400	0.31187700
H	-2.40595700	2.37985800	2.56479300
H	-0.76665400	3.03413800	2.46747800
H	-1.02588800	1.27224100	2.34476100
O	2.42147800	0.45221600	-1.14155200
C	2.24594200	1.55114300	-2.03589900
C	3.79338500	0.25727000	-0.82792800
C	3.64636300	1.88112800	-2.54503700
C	4.51158100	1.50423100	-1.34106000
H	4.48219400	2.30606100	-0.58736500
H	5.56270000	1.31403400	-1.59383400
H	3.88207300	0.09868300	0.25808800
H	4.16438500	-0.64717000	-1.34332500
H	1.79011500	2.39359900	-1.48854400
H	1.54701400	1.24958800	-2.82788600
H	3.89921800	1.24492600	-3.40676600
H	3.74986200	2.92978100	-2.85111300
H	1.16202800	2.16196700	1.17049500
C	2.07818000	1.83097800	1.68423500
O	2.00128800	0.41500300	1.86610700
H	1.68553700	3.39803900	3.17083200
C	2.21121600	2.43807000	3.08420500
H	2.93646600	2.06909000	1.03690000
H	1.41854600	-0.78400500	3.42030800
C	2.06912000	0.08345200	3.24926300
H	0.53091200	1.40574900	3.99605300
C	1.62788800	1.34392100	3.98117000
H	3.27018100	2.60671200	3.33092600
H	3.10849700	-0.18506800	3.51521900
H	1.99547100	1.38611500	5.01458600
C	2.53322800	-2.85290200	0.95423900
O	1.86514100	-2.31263700	-0.17808600
C	2.31260600	-2.93757800	-1.37793300
C	3.35064000	-3.97980000	-0.94909500
C	3.82699600	-3.43371500	0.39831000
H	2.68027400	-2.04214500	1.68068300

H	1.90872400	-3.63312000	1.42316900
H	1.45487200	-3.37954200	-1.90462100
H	2.74275200	-2.15953400	-2.03035100
H	2.87177300	-4.95982400	-0.80721100
H	4.15584800	-4.10027500	-1.68527800
H	4.26943900	-4.19810700	1.05007100
H	4.56766200	-2.63273300	0.25141700

Table S89. Atomic coordinates and single point energies for **76**.

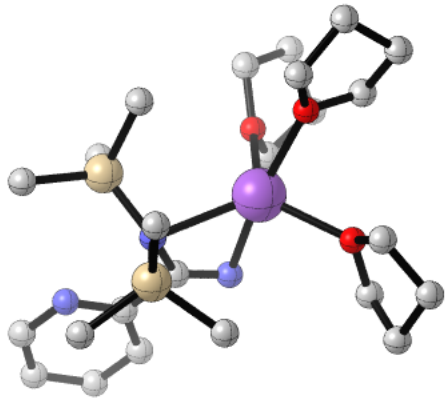


G = –1839.033016
G_{SP} = –1840.537153

N	3.66560700	-0.27306400	-0.16799200
C	4.99551100	-0.19349300	-0.21879600
C	2.94633200	0.82720000	-0.39763300
C	5.68341700	0.98479000	-0.49194900
C	3.54971400	2.05948700	-0.69522700
C	4.93362800	2.13812100	-0.73643600
H	5.54519000	-1.12216000	-0.03112200
H	6.77339200	0.99561500	-0.51545500
H	5.42987900	3.08494500	-0.95899100
H	2.88994600	2.90588600	-0.88444300
C	1.42991400	0.77534000	-0.36310100
N	0.68824800	1.72075900	-0.66741200
Na	-1.21461800	0.49401400	-0.47996000
N	0.91317800	-0.58093800	0.14025300
Si	1.15538600	-1.99229800	-0.88257900
Si	0.72182800	-0.57186100	1.88298300
C	2.30519800	-3.31835100	-0.19849200
C	1.72077300	-1.41766400	-2.58198200
C	-0.52652300	-2.84411800	-1.14943400
C	2.21783000	0.14931600	2.76129800
C	0.40435900	-2.30521800	2.55781900
C	-0.76037400	0.53399100	2.31788700
H	-0.92358600	-3.26196300	-0.21092900
H	-0.41804600	-3.67955800	-1.85946900
H	-1.28180100	-2.15394000	-1.56162000
H	3.19231100	-2.84485000	0.24349700

H	2.63318500	-3.98185100	-1.01419800
H	1.80942600	-3.94244800	0.55918800
H	2.76088200	-1.06498700	-2.56190700
H	1.09191800	-0.59116100	-2.94724700
H	1.64896000	-2.24989700	-3.29915600
H	-0.60801700	1.52752200	1.86397400
H	-0.83962600	0.67043400	3.40725600
H	-1.72593500	0.12654500	1.97189300
H	1.33558200	-2.88965300	2.57753900
H	-0.33621900	-2.87167500	1.97336800
H	0.03287600	-2.23136700	3.59183800
H	3.11394400	-0.44962300	2.54379100
H	2.05626400	0.16846900	3.85032200
H	2.41202900	1.17839000	2.42239000
O	-3.09245000	-0.71369200	-0.16935700
C	-3.34813500	-1.76857200	0.75734700
C	-4.01314600	-0.76629200	-1.26409100
C	-4.19969200	-2.76966500	-0.01049100
C	-5.03523800	-1.83564700	-0.88748000
H	-5.85405300	-1.39400900	-0.29984000
H	-5.47087400	-2.32803200	-1.76588300
H	-4.44092000	0.23490900	-1.41327400
H	-3.46135800	-1.04518200	-2.17814800
H	-3.89077200	-1.36455800	1.63007700
H	-2.38472600	-2.17011600	1.10187700
H	-3.55404600	-3.40674000	-0.63411900
H	-4.79848300	-3.41303400	0.64638100
H	-3.80625700	1.58923500	0.72952500
C	-3.55662700	2.51845300	0.19731700
O	-2.67994700	2.18297200	-0.86563400
H	-2.42114600	3.10600500	1.97768700
C	-2.80378200	3.55677000	1.05261000
H	-4.48607400	2.94915500	-0.21738400
H	-1.09210400	3.10551600	-1.78072400
C	-1.98879500	3.38133400	-1.21325400
H	-0.68368100	3.60663900	0.46114800
C	-1.64964200	4.01699400	0.13310300
H	-3.46747100	4.38396300	1.33725400
H	-2.65679200	4.02025300	-1.81953600
H	-1.56238700	5.10919200	0.07022200

Table S90. Atomic coordinates and single point energies for **75**.



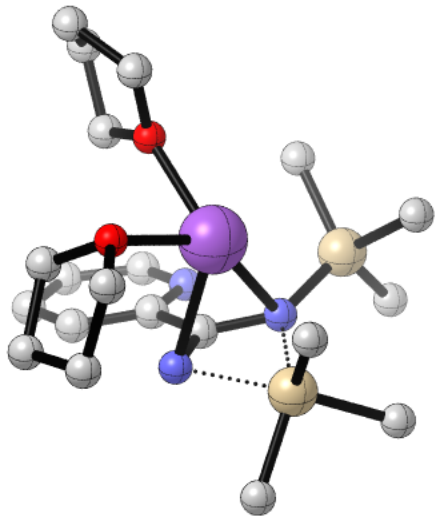
G = –2071.103551
G_{SP} = –2072.859828

N	-4.00330800	0.29811400	-0.04183200
C	-5.30352100	0.43494500	-0.30242700
C	-3.17592600	-0.02294400	-1.03956100
C	-5.85598000	0.25345600	-1.56657600
C	-3.63946200	-0.21630500	-2.35153700
C	-4.99400400	-0.08085800	-2.61464900
H	-5.94302500	0.70347100	0.54559500
H	-6.92838100	0.37229600	-1.72363400
H	-5.38197000	-0.23186000	-3.62421600
H	-2.89787700	-0.46524300	-3.11029000
C	-1.68737100	-0.17414100	-0.78189500
N	-0.83581400	-0.34705100	-1.66571100
Na	0.92919700	-0.09289800	-0.19467600
N	-1.35979100	-0.13959900	0.71380700
Si	-1.53740600	1.38426600	1.57906200
Si	-1.52697200	-1.69539800	1.50765600
C	-2.84802200	1.36341200	2.93400200
C	-1.86755200	2.77785500	0.36184700
C	0.11105400	1.77661700	2.44070400
C	-0.85800800	-3.02095500	0.34680800
C	-3.29225800	-2.15494400	1.97413200
C	-0.46362800	-1.70660700	3.07318800
H	0.31981000	1.05360800	3.24432100
H	0.08356800	2.78095500	2.89326300
H	0.95170100	1.74974200	1.72875200
H	-3.82730200	1.13812900	2.49001000
H	-2.89581400	2.34452900	3.43203100
H	-2.63116600	0.60847100	3.70568500

H	-2.88439100	2.72284000	-0.04964000
H	-1.15029900	2.71015200	-0.46907400
H	-1.74142300	3.75187400	0.86028700
H	0.58677400	-1.46925600	2.83679000
H	-0.48909700	-2.70495700	3.53706700
H	-0.81321600	-0.98241800	3.82454300
H	-3.91185600	-2.25769200	1.07143400
H	-3.75171600	-1.37942200	2.60352500
H	-3.30994400	-3.11070100	2.52157200
H	-1.47535100	-3.08692300	-0.56167600
H	-0.84258600	-4.00522400	0.84036500
H	0.16292400	-2.76680500	0.02379400
O	2.94366800	0.30035300	0.85980600
C	3.46273600	0.17783200	2.18118000
C	3.99263600	0.55397800	-0.07686500
C	4.86203900	0.77752200	2.11602900
C	5.29202200	0.37407900	0.70507800
H	5.60757300	-0.68067500	0.69413800
H	6.11414500	0.97934000	0.30242600
H	3.87707900	-0.13655400	-0.92441100
H	3.89212800	1.58481900	-0.45582500
H	3.50174000	-0.88926200	2.46362800
H	2.78521800	0.69781700	2.87226300
H	4.80952600	1.87380400	2.20096600
H	5.52483300	0.40198800	2.90594200
H	2.40306000	-3.04815000	0.57901000
C	2.94135700	-2.76516600	-0.34311000
O	2.15863500	-1.82631500	-1.06943200
H	3.24389000	-4.90790400	-0.72386700
C	3.12256500	-3.96516400	-1.27272500
H	3.89399100	-2.29465900	-0.05038600
H	0.63156100	-2.05721200	-2.42232700
C	1.66839900	-2.39815000	-2.29102900
H	0.99692200	-4.32179500	-1.56087200
C	1.84778700	-3.90119900	-2.11707900
H	4.00817800	-3.82304300	-1.91061200
H	2.28030000	-2.02082300	-3.12946000
H	1.93192100	-4.43108900	-3.07457600
C	0.88349200	2.26964500	-2.28193300
O	1.21802100	2.03705100	-0.91929600
C	1.79594100	3.23169400	-0.43036800
C	2.55748400	3.85329200	-1.62472700
C	2.11664700	2.98719100	-2.82398700
H	0.62939500	1.30479100	-2.73770500

H	-0.00917500	2.92084800	-2.33562500
H	0.99660000	3.90441600	-0.07167100
H	2.43520000	2.97111900	0.42547200
H	2.27429700	4.90561100	-1.75904900
H	3.64603200	3.82480000	-1.47969400
H	1.90441700	3.57642600	-3.72504800
H	2.89115600	2.24807200	-3.07534400

Table S91. Atomic coordinates and single point energies for **TS-16**.

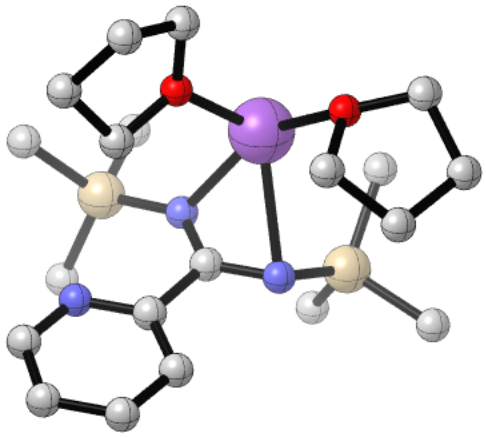


G = –1839.002191
G_{SP} = –1840.497489

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.33230061
C	1.17018497	0.00000000	-0.63747287
C	1.16458616	-0.00235375	2.09739953
C	2.39697762	-0.03601633	0.04243296
C	2.39138022	-0.02844869	1.43056176
H	-0.98094980	0.00105146	1.81840842
H	1.10807077	-0.00031666	3.18615026
H	3.32764078	-0.05167937	1.99131775
H	3.31072897	-0.08277370	-0.55053826
C	1.17395355	-0.01166309	-2.13747225
N	2.22194303	-0.17059729	-2.84803661
N	-0.00913873	0.09882767	-2.88345722
Si	0.91779578	-0.65706347	-4.38167874
C	2.07867864	-2.14847344	-4.68277909
C	1.30128353	0.71596851	-5.67157994
C	-0.65078099	-1.51032608	-5.13379661
Si	-1.63512804	0.69295379	-2.59895921
C	-1.77993685	2.11784775	-1.35838587
C	-2.83871372	-0.67323863	-2.14385725
C	-2.16718401	1.57153700	-4.19774273
H	2.29878711	1.17197618	-5.56285025
H	0.53170890	1.50890502	-5.69600581
H	1.27921111	0.25311925	-6.66918645
H	-0.83787033	-2.43402089	-4.55844667

H	-0.45780184	-1.82228164	-6.17368060
H	-1.58584420	-0.93422037	-5.12230745
H	3.13243274	-1.83564893	-4.70451352
H	1.82667280	-2.68624251	-5.61000151
H	1.97725009	-2.85821231	-3.84542781
H	-1.71438707	1.79211339	-0.31331034
H	-2.75671247	2.60367346	-1.51578975
H	-1.00341441	2.87754693	-1.54659110
H	-2.51863629	-1.12675527	-1.19440082
H	-2.84461441	-1.45729777	-2.91486780
H	-3.86374552	-0.29047309	-2.02519975
H	-1.59293143	2.50969742	-4.29869725
H	-3.22921196	1.85692603	-4.13099824
H	-2.02851560	0.99454814	-5.12006567
Na	1.53189272	2.07821903	-3.45248430
O	3.68003922	2.76116278	-3.67561865
C	4.54485317	2.47086238	-4.76615643
C	5.04128575	1.06085098	-4.47241835
C	5.17770408	1.06352032	-2.93846449
C	4.33223001	2.27406022	-2.49956571
H	5.37655692	3.19936926	-4.78158132
H	3.97216003	2.57400714	-5.69745629
H	5.97682302	0.82269703	-4.99438817
H	4.27247782	0.33146591	-4.76623361
H	6.22259229	1.17796569	-2.61945634
H	4.75833386	0.13821611	-2.52637991
H	4.95633673	3.08259143	-2.07924756
H	3.55442199	2.00521403	-1.77188043
O	1.44603418	3.53162596	-1.73512622
C	1.42878610	3.34419199	-0.31578642
C	1.77163158	4.88944972	-2.05896800
C	1.26441206	4.74452840	0.25458907
C	2.09932739	5.56515247	-0.72902924
H	0.20691255	5.04689613	0.21140467
H	1.60633111	4.82144207	1.29435926
H	0.61217827	2.65408162	-0.06555463
H	2.38277008	2.89030300	0.00530702
H	0.89404608	5.35296787	-2.53909270
H	2.61120424	4.88756904	-2.76945018
H	3.16963890	5.45605177	-0.49823166
H	1.85694296	6.63528980	-0.73191035

Table S92. Atomic coordinates and single point energies for **77**.

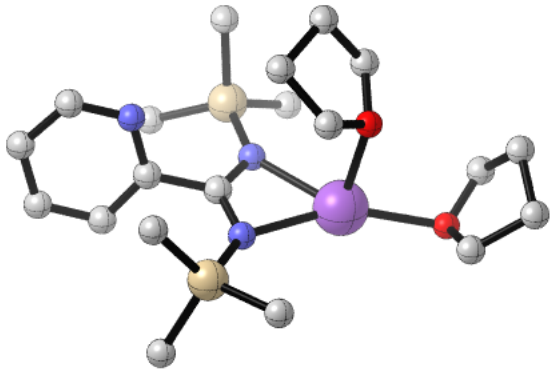


G = –1839.051189
G_{SP} = –1840.546333

N	-2.63553000	-0.00230700	1.26897000
C	-3.43237500	0.46297100	2.22648300
C	-1.39994500	-0.39053100	1.58522500
C	-3.03693100	0.57908400	3.55864100
C	-0.91483300	-0.32325700	2.89808800
C	-1.74601800	0.17448500	3.89590000
H	-4.44010400	0.76270800	1.91957800
H	-3.72635300	0.97188800	4.30643500
H	-1.39539200	0.24176700	4.92757000
H	0.10082600	-0.66909500	3.08396700
C	-0.50422700	-0.91100200	0.46152300
N	0.74034500	-1.19893800	0.83364700
N	-0.95662400	-0.97906400	-0.77294500
Si	1.60932200	-2.49668500	0.08766600
C	2.99288500	-3.03295300	1.25278400
C	2.43121300	-2.06580200	-1.58677600
C	0.49958300	-3.98556200	-0.22987000
Si	-2.49898300	-1.07353700	-1.55467100
C	-3.37010600	0.57807300	-1.87893200
C	-3.69384500	-2.30330600	-0.76783100
C	-2.08515500	-1.74451800	-3.27788500
H	3.06297000	-1.16300300	-1.53509300
H	1.67501700	-1.94170200	-2.38149800
H	3.08549700	-2.89195000	-1.90491600
H	0.03566800	-4.32000800	0.71056100
H	1.06474600	-4.82923000	-0.65471100
H	-0.30426500	-3.71014700	-0.92789300

H	3.70832000	-2.22523300	1.46617600
H	3.55434900	-3.88342700	0.83627100
H	2.55753800	-3.34886700	2.21297100
H	-3.78835300	1.00721000	-0.95787300
H	-4.18948900	0.42815900	-2.59961200
H	-2.66860600	1.30462000	-2.32139000
H	-4.08140200	-1.93643200	0.19176200
H	-3.18172400	-3.26157200	-0.58913300
H	-4.54394600	-2.49586000	-1.44103100
H	-1.40197700	-1.05679300	-3.80341400
H	-2.98151600	-1.87153800	-3.90469900
H	-1.57906700	-2.71947300	-3.20072600
Na	0.94004600	0.21584400	-1.31643500
O	2.79369200	1.31727300	-0.60289800
C	4.20251100	1.19745400	-0.70436400
C	4.62839000	0.44184800	0.55933300
C	3.49976400	0.76242000	1.56669700
C	2.52428100	1.62839100	0.76215300
H	4.65159700	2.20680100	-0.73653200
H	4.43953000	0.68029700	-1.64357400
H	5.61967300	0.76005900	0.90661000
H	4.67499500	-0.63733500	0.35824500
H	3.86476100	1.28479800	2.46018000
H	2.97664000	-0.15110500	1.88135500
H	2.69575200	2.70908000	0.92393100
H	1.47561000	1.38330100	0.97424800
O	0.05517900	2.27110600	-1.07716100
C	-0.97199800	2.49841200	-0.10741000
C	0.59298100	3.50891100	-1.54272400
C	-1.41454200	3.93330900	-0.34718200
C	-0.08393700	4.59618600	-0.70809100
H	-2.11266000	3.97441600	-1.19741100
H	-1.90568600	4.37832700	0.52736300
H	-1.75293800	1.74225500	-0.24658900
H	-0.55359300	2.37785300	0.91009800
H	0.35165000	3.61710400	-2.61298300
H	1.68718100	3.48309000	-1.43084700
H	0.49650900	4.79438900	0.20579700
H	-0.19148100	5.54092900	-1.25614800

Table S93. Atomic coordinates and single point energies for **78**.

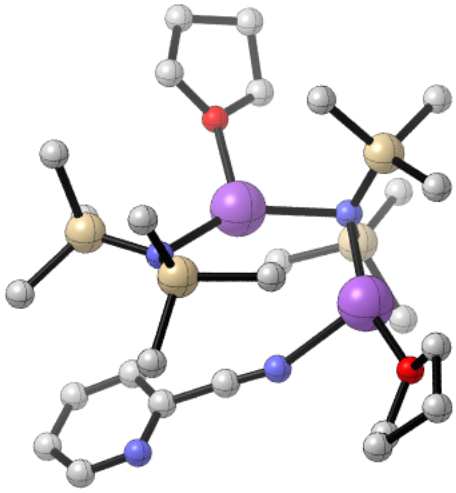


G = –1839.066163
G_{SP} = –1840.561724

N	2.77804700	-0.48782900	1.02826000
C	4.05073100	-0.52070200	1.41947700
C	2.49399400	0.06194000	-0.15371600
C	5.10489600	-0.03271300	0.64851200
C	3.48072500	0.57911000	-1.00258700
C	4.80846800	0.52179900	-0.59643900
H	4.24627800	-0.96683600	2.39954800
H	6.12971500	-0.09448200	1.01490700
H	5.60398500	0.90218500	-1.23988600
H	3.19137000	1.00407400	-1.96450500
C	1.03459700	0.10047000	-0.56072200
N	0.44856400	1.28530500	-0.65540300
N	0.41122500	-1.03827900	-0.79282800
Si	1.00723600	2.86652600	-0.23040200
C	2.00465500	2.91332400	1.37808300
C	-0.54333700	3.92523900	-0.00187900
C	2.02121700	3.71084700	-1.58650600
Si	1.05125400	-2.64851300	-0.85640100
C	1.05822100	-3.51247500	0.82679000
C	2.79730700	-2.78147100	-1.57477000
C	-0.10742000	-3.61971900	-1.98728800
H	-1.18141000	3.55252400	0.81433700
H	-1.14125900	3.91977700	-0.92730700
H	-0.28581600	4.97072300	0.22696800
H	3.05340900	3.33380700	-1.62601400
H	2.06965400	4.79615300	-1.40585600
H	1.55793400	3.55053100	-2.57211400
H	1.50100100	2.33125000	2.16614100
H	2.12443000	3.94763600	1.73674200

H	3.00932700	2.48300100	1.24231100
H	1.55725000	-2.87585100	1.57289300
H	1.60143300	-4.46861000	0.76352600
H	0.03846800	-3.73594600	1.17615400
H	3.56631800	-2.42279900	-0.87346800
H	2.88692300	-2.19793900	-2.50416600
H	3.02097200	-3.83385300	-1.81151500
H	-1.14150100	-3.57846900	-1.60888400
H	0.18351400	-4.67900600	-2.05868800
H	-0.10547700	-3.19313700	-3.00202200
Na	-1.53684900	0.19565800	-0.99663700
O	-3.74365600	0.26875400	-1.45831400
C	-4.43320200	-0.90597600	-1.02676700
C	-5.31198800	-0.45909700	0.13535000
C	-5.65144000	0.97376000	-0.27652700
C	-4.32579900	1.43536900	-0.87087000
H	-3.69292700	-1.67045300	-0.74353400
H	-5.03275400	-1.29846400	-1.86477600
H	-4.71873500	-0.44829000	1.06122600
H	-6.19175500	-1.10006600	0.27431500
H	-5.98118000	1.60465400	0.55843500
H	-6.43821200	0.97824200	-1.04584700
H	-3.65427300	1.81768900	-0.08146400
H	-4.43329600	2.20450200	-1.64785500
O	-2.21248200	-0.21306900	1.17699600
C	-1.47783800	0.62348700	2.07839700
C	-2.07096500	-1.58704200	1.55644900
C	-0.46994200	-0.30012300	2.74500000
C	-1.28726700	-1.58656100	2.86804000
H	0.40208700	-0.45284200	2.08874300
H	-0.11771800	0.08627100	3.71053700
H	-1.00664100	1.42518500	1.49476400
H	-2.17516400	1.06411900	2.81339200
H	-1.51331900	-2.10858200	0.76138800
H	-3.07222700	-2.03679400	1.65385800
H	-1.97428600	-1.52541000	3.72607400
H	-0.66906300	-2.48556800	2.98207900

Table S94. Atomic coordinates and single point energies for **79**.



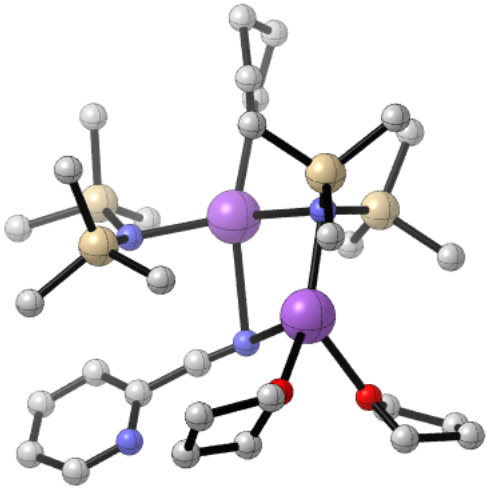
G = –2873.865458
G_{SP} = –2875.963605

N	-4.37658900	0.39783700	1.65313700
C	-5.40401200	-0.39166600	1.94242600
C	-3.15545600	-0.09606600	1.84585600
C	-5.25575600	-1.68558000	2.45095600
C	-2.88451400	-1.37247200	2.34131800
C	-3.97210500	-2.18228300	2.65443500
H	-6.39955100	0.02391500	1.76581300
H	-6.13601700	-2.28895100	2.67278000
H	-3.81517400	-3.19117300	3.03832900
H	-1.85509000	-1.71030400	2.45894600
C	-2.04764500	0.79966600	1.56339200
N	-1.16195700	1.52384900	1.41704200
Na	0.84588100	2.41666600	0.50462100
Na	0.70282800	-0.99170400	-0.09483500
N	-1.39705700	-1.07700300	-0.94911500
N	2.27755800	0.60317200	0.61785800
Si	-1.99088900	-2.66781500	-1.05280200
Si	-1.85904000	0.17417500	-2.00151400
C	-3.88941300	-2.78596000	-0.99179300
C	-1.33010300	-3.75579200	0.37579600
C	-1.50225200	-3.59346000	-2.64686900
C	-3.56431400	0.94676600	-1.67030500
C	-1.89039200	-0.30428300	-3.84218600
C	-0.65679800	1.66652400	-1.89314000
Si	2.43282400	0.36013500	2.29585000

Si	3.38115800	0.88741700	-0.64668500
C	1.21074600	-0.98896300	2.85424100
C	1.94376400	1.92656100	3.26767400
C	4.14607900	-0.12177600	2.94590800
C	3.20341100	2.67399400	-1.29672900
C	3.02691300	-0.25110000	-2.12595000
C	5.21602400	0.67483600	-0.22537900
H	-4.30003400	-2.15288000	-0.18946000
H	-4.24139200	-3.81858000	-0.83542300
H	-4.31772900	-2.42831800	-1.94257200
H	-1.94384000	-3.65720800	1.28327900
H	-0.28848900	-3.51284400	0.64659200
H	-1.35818700	-4.81984900	0.08942300
H	-2.05053500	-3.19423800	-3.51329400
H	-1.72787800	-4.67016700	-2.57599200
H	-0.42937100	-3.47923600	-2.86560100
H	-4.35715400	0.18341600	-1.72146500
H	-3.79278900	1.71828900	-2.42453600
H	-3.63014100	1.41458800	-0.67523800
H	-2.70377900	-1.01950200	-4.04423300
H	-0.94602300	-0.78172800	-4.14835000
H	-2.05755000	0.57610900	-4.48319900
H	-0.96606900	2.33553400	-1.07394600
H	-0.68505400	2.25228800	-2.82602000
H	0.38761000	1.34442900	-1.74093100
H	0.18403900	-0.66766200	2.61109100
H	1.25083600	-1.16332100	3.94030800
H	1.40017100	-1.95356900	2.35380200
H	0.87730400	2.17867100	3.13960400
H	2.54921300	2.78841100	2.93824400
H	2.11089400	1.80462100	4.34906900
H	4.52785400	-1.04590700	2.48662000
H	4.09841800	-0.28385900	4.03442200
H	4.88255700	0.67350300	2.75663300
H	3.67536200	-0.01730100	-2.98444000
H	1.98238000	-0.17141000	-2.47323700
H	3.20095700	-1.30239000	-1.84722500
H	2.21287900	2.84896700	-1.75072900
H	3.94884300	2.90112900	-2.07456300
H	3.34925200	3.40353300	-0.48077500
H	5.53735400	1.40609900	0.53215800
H	5.83368200	0.82758400	-1.12445900
H	5.43768300	-0.32918200	0.16894900
O	2.00512200	-2.86883400	-0.17860400

C	3.29337400	-2.90211700	0.43736100
C	1.90533800	-3.86479500	-1.19977100
C	4.14958100	-3.79222600	-0.45702400
C	3.10953200	-4.77690200	-0.99278100
H	2.88271800	-5.54187400	-0.23502500
H	3.41636600	-5.28530300	-1.91553200
H	0.93699000	-4.37448300	-1.10173400
H	1.94058600	-3.37088600	-2.18644500
H	4.57905300	-3.20324800	-1.28214500
H	4.97300000	-4.27051400	0.08848000
H	3.66264300	-1.87002000	0.52450200
H	3.19953600	-3.32619300	1.45216800
O	0.08178500	4.47267900	0.01981400
C	-1.22582100	4.85418600	0.46437300
H	-1.12749400	5.56603000	1.30091300
H	-1.75042300	3.95773400	0.82278000
C	-1.88083800	5.50508200	-0.74598400
H	-2.68647500	6.19691200	-0.46988200
H	-2.29740300	4.73288800	-1.41069500
C	-0.68186400	6.18641100	-1.40551600
H	-0.43020100	7.11576300	-0.87281200
H	-0.83902300	6.42787900	-2.46423400
C	0.41073500	5.14155400	-1.20373400
H	1.42031500	5.56631600	-1.11640900
H	0.40761100	4.40155400	-2.02138600

Table S95. Atomic coordinates and single point energies for **80**.



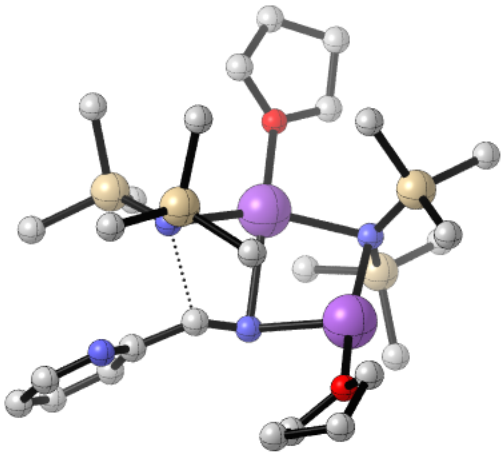
G = –3105.936285
G_{SP} = –3108.296925

N	-1.22528100	4.08789100	-0.99027200
C	-1.01253300	5.39899600	-0.97115200
C	-0.22127800	3.31125700	-1.40104000
C	0.19369400	5.98076400	-1.37125800
C	1.02629500	3.77710300	-1.81479200
C	1.22678700	5.15463800	-1.80331000
H	-1.84012300	6.02085600	-0.61928600
H	0.31500000	7.06343000	-1.33447800
H	2.18552500	5.57268100	-2.11286700
H	1.80023000	3.06956000	-2.10409800
C	-0.51626000	1.89025900	-1.39091900
N	-0.85795500	0.78809700	-1.37576900
Na	-2.06390800	-0.56491200	0.27068700
Na	1.23367100	-0.66633800	-0.34507100
N	2.16070800	1.39771900	0.08633400
N	-0.35984900	-2.21479000	0.43020700
Si	3.69659800	1.47031700	-0.62704500
Si	1.65210600	2.05353700	1.56282400
C	4.47199400	3.20975400	-0.71173200
C	3.58949200	0.83261100	-2.42153200
C	5.02514100	0.40898500	0.22283800
C	1.52820200	3.95455500	1.63520000
C	2.74887200	1.58533300	3.04398500
C	-0.12295600	1.45370200	1.95797200
Si	-0.50240100	-3.25162400	-0.92248600
Si	-0.55007200	-2.66391900	2.06872300

C	0.06799300	-2.35506700	-2.50380200
C	-2.29866600	-3.81801500	-1.21444700
C	0.54277000	-4.83447000	-0.90506100
C	-0.69319300	-4.52422800	2.41335800
C	-2.14739200	-1.87382200	2.76689100
C	0.81914600	-2.03884500	3.22443600
H	3.80729200	3.95119400	-1.18173200
H	5.41906600	3.19760300	-1.27453000
H	4.69437600	3.57111200	0.30563000
H	2.98957700	1.49253600	-3.06963700
H	3.11319500	-0.16219800	-2.44917900
H	4.58467900	0.73675000	-2.88423300
H	5.19084300	0.74953900	1.25687500
H	5.98961000	0.44678000	-0.30914300
H	4.69424500	-0.63872400	0.26639100
H	2.45690300	4.42664700	1.27639600
H	1.35548200	4.29302200	2.66974800
H	0.69813600	4.33663600	1.01945000
H	3.72351200	2.09369400	2.95728200
H	2.94633400	0.50220200	3.07399400
H	2.30323900	1.88135400	4.00707500
H	-0.86329400	1.97092700	1.32373500
H	-0.38962600	1.64243700	3.01071300
H	-0.21426100	0.36754400	1.78741400
H	-0.36300500	-1.34892000	-2.61558800
H	-0.19543900	-2.93882100	-3.39984800
H	1.16618800	-2.25409500	-2.49799700
H	-2.98540900	-2.95684600	-1.23539400
H	-2.62495300	-4.47600900	-0.39264600
H	-2.41394900	-4.37647600	-2.15761600
H	1.61055800	-4.57165400	-0.85118800
H	0.38250800	-5.40213800	-1.83582500
H	0.30318200	-5.49601500	-0.06033800
H	-3.03670400	-2.13121300	2.16362600
H	-2.04614800	-0.77543500	2.80047600
H	-2.34424400	-2.20574100	3.79796200
H	-1.47292000	-5.00402500	1.80125400
H	-0.94021200	-4.69567800	3.47296900
H	0.25900400	-5.03745900	2.20733800
H	1.71803500	-2.67057900	3.16590300
H	0.47220800	-2.06125200	4.26996200
H	1.11696600	-1.00335100	2.99644800
O	2.91320700	-2.22365500	-0.60610000
C	3.15120100	-2.74998000	0.70297500

C	3.88308800	-2.70685100	-1.53100200
C	4.49360700	-3.47372800	0.62108900
C	4.53238000	-3.90493300	-0.84641200
H	3.92454300	-4.80946900	-0.99853500
H	5.54600100	-4.10309600	-1.21785500
H	3.37364900	-2.96065000	-2.47260700
H	4.62168600	-1.91178500	-1.73311600
H	5.31796800	-2.77669000	0.83344700
H	4.55939300	-4.31153500	1.32678000
H	3.14996400	-1.91680400	1.42362000
H	2.32376300	-3.43247700	0.95928500
O	-3.54493000	0.91200900	1.23396400
C	-4.13655400	1.14992200	2.50054800
H	-3.81835800	0.35817900	3.18891500
H	-5.23782700	1.11148700	2.39883800
C	-3.67028700	2.55589000	2.88356300
H	-2.70847900	2.49876200	3.40954100
H	-4.38865500	3.06332700	3.54003500
C	-3.49685500	3.25311800	1.51565700
H	-2.49203500	3.68131600	1.40675200
H	-4.22228800	4.06272600	1.36127400
C	-3.71306800	2.11920600	0.49935100
H	-2.99962800	2.13388700	-0.33356200
H	-4.73821700	2.14693200	0.08721400
C	-3.51808800	-0.76823900	-2.68604700
O	-3.71188500	-0.56177400	-1.29241900
C	-5.10683600	-0.60920600	-1.05460400
C	-5.58959400	-1.77710800	-1.91137000
C	-4.65785700	-1.70603400	-3.13925800
H	-3.56478300	0.20437800	-3.20512400
H	-2.51463300	-1.19025300	-2.82567800
H	-5.26573400	-0.72549500	0.02514600
H	-5.57311800	0.33975900	-1.38133900
H	-5.44004400	-2.72077300	-1.36860300
H	-6.65280800	-1.69717900	-2.17137500
H	-4.27754200	-2.69953100	-3.40803500
H	-5.17300500	-1.29595400	-4.01784400

Table S96. Atomic coordinates and single point energies for **TS-10**.



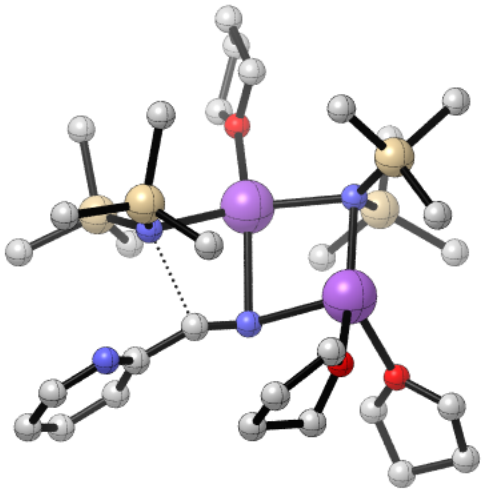
G = –2873.855561
G_{SP} = –2875.950672

N	-4.10645700	0.07440600	-0.44870300
C	-5.35075700	0.42113600	-0.75493400
C	-3.16205400	0.29395100	-1.35860700
C	-5.71254400	0.98916900	-1.97959300
C	-3.41056200	0.83631500	-2.62344600
C	-4.72016800	1.19344200	-2.93319900
H	-6.10728200	0.23912700	0.01426900
H	-6.75029200	1.26020600	-2.17331700
H	-4.95885800	1.62687100	-3.90546900
H	-2.59365500	0.96382800	-3.33391900
C	-1.80385300	-0.16469500	-1.05185100
N	-0.91838300	-0.90041900	-1.25966000
Na	0.59914000	-2.49383000	-0.52711700
Na	0.81140100	0.78187500	-0.21403400
N	-1.34703600	1.32494100	0.58172500
N	2.34966200	-0.98567200	-0.53748100
Si	-1.70967100	2.96819800	0.24439400
Si	-1.55629100	0.58420600	2.11602700
C	-3.54763700	3.36051000	-0.03011400
C	-0.79618200	3.46702100	-1.34475900
C	-1.22160400	4.16822500	1.63718500
C	-3.31148600	0.62147200	2.82301600
C	-0.45294500	1.34675200	3.46548500
C	-1.04065900	-1.24896200	2.00893600
Si	2.66592100	-0.90800000	-2.20746700
Si	3.26391100	-1.39700400	0.83395300

C	1.78281300	0.58559000	-2.98924200
C	1.94534400	-2.42956900	-3.11250500
C	4.48722800	-0.81217000	-2.72103300
C	2.73990500	-3.11592800	1.48755100
C	2.92124500	-0.18900400	2.25532600
C	5.14367100	-1.47544800	0.60447900
H	-3.94192500	2.95714200	-0.97358200
H	-3.69927600	4.45186700	-0.04581800
H	-4.15138400	2.94720200	0.79349800
H	-1.11645000	2.82296500	-2.18095900
H	0.29682600	3.35613900	-1.24558200
H	-1.00542800	4.50935600	-1.63173100
H	-1.95494400	4.09820600	2.45727800
H	-1.23182400	5.20938200	1.27540000
H	-0.23198700	3.95591200	2.06411400
H	-3.63717600	1.66243100	2.98151300
H	-3.35902400	0.10557100	3.79523000
H	-4.01544000	0.14429500	2.12669500
H	-0.86408600	2.30786400	3.80912700
H	0.56962100	1.53341900	3.10116700
H	-0.38210000	0.68105600	4.34101300
H	-1.67921000	-1.79863800	1.30070400
H	-1.11416800	-1.72835000	2.99818400
H	0.00972400	-1.33839500	1.67748400
H	0.68942000	0.47928300	-2.89140900
H	2.00587300	0.66229900	-4.06467500
H	2.07999600	1.53892600	-2.52238400
H	0.84179400	-2.44027000	-3.07479200
H	2.32510500	-3.36805300	-2.67254400
H	2.21950200	-2.43723600	-4.17872700
H	4.99853600	0.05064400	-2.26708000
H	4.56775100	-0.71313600	-3.81506800
H	5.03582500	-1.71822100	-2.42299300
H	3.54859100	-0.38947000	3.13765300
H	1.86947600	-0.25536300	2.57770600
H	3.10078500	0.84993700	1.93383000
H	1.68820500	-3.11411700	1.82578200
H	3.34337000	-3.43288700	2.35229500
H	2.85506800	-3.88710700	0.70588500
H	5.42848000	-2.25937000	-0.11369200
H	5.63671100	-1.70054000	1.56331600
H	5.55163200	-0.52222800	0.23272700
O	2.38218400	2.45826300	-0.01614700
C	3.73610400	2.26500200	-0.43129200

C	2.28211500	3.57525600	0.87011900
C	4.57566800	3.06921900	0.55279800
C	3.65039800	4.25190700	0.84037900
H	3.69885500	4.97997000	0.01684300
H	3.87950800	4.77628600	1.77664800
H	1.46341200	4.22683300	0.53326100
H	2.03684100	3.20515700	1.88059700
H	4.75095100	2.48527600	1.46938000
H	5.54899500	3.36076900	0.13789400
H	3.94329700	1.18598900	-0.42750100
H	3.86033700	2.64339900	-1.46123100
O	-0.82202000	-4.10220900	0.09938800
C	-2.18180900	-4.05055200	-0.35292100
H	-2.28564200	-4.70264600	-1.23570900
H	-2.41907600	-3.01777500	-0.64650300
C	-3.01567600	-4.55725900	0.81807400
H	-3.96600200	-5.00119000	0.49593900
H	-3.23582000	-3.73194400	1.51178000
C	-2.05882000	-5.55585000	1.46942600
H	-2.04331800	-6.49894500	0.90259800
H	-2.30446600	-5.78405700	2.51420500
C	-0.72724400	-4.82874600	1.32878700
H	0.14254500	-5.49794600	1.27584600
H	-0.57709700	-4.11373600	2.15531300

Table S97. Atomic coordinates and single point energies for **TS-15**.



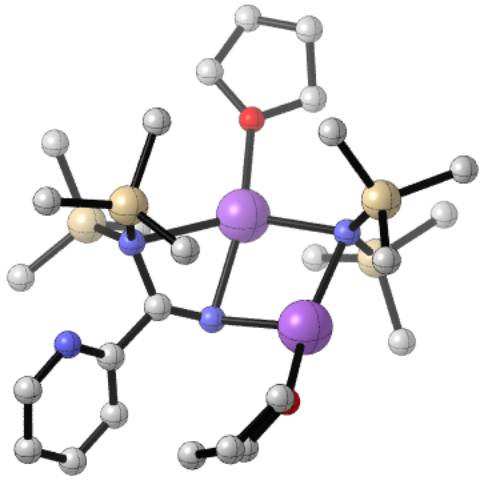
G = –3105.933339
G_{SP} = –3108.290578

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.32668799
C	1.17697033	0.00000000	-0.62081698
C	1.16700878	0.00774975	2.09690498
C	2.40507833	0.04283798	0.04631647
C	2.39180445	0.03947226	1.43908394
H	-0.98121961	-0.00795681	1.81051384
H	1.10631594	-0.00555955	3.18496248
H	3.32774108	0.05821978	1.99918757
H	3.33547966	0.07553323	-0.52004191
C	1.17470741	0.05276249	-2.08459687
N	1.37745062	0.56959155	-3.11176075
Na	0.62748597	1.44828543	-5.16614521
Na	1.17177418	-1.62574922	-4.46796167
N	0.35094672	-2.09347218	-2.33649248
N	0.93310317	-0.46782004	-6.48702633
Si	1.33431926	-3.31616022	-1.66135600
Si	-1.36045285	-2.08031262	-2.38492585
C	1.21555649	-3.47395119	0.22704374
C	3.15506106	-2.94264620	-2.06581678
C	0.95565754	-5.04809487	-2.34578047
C	-2.24307386	-2.48084037	-0.75542632
C	-2.06532369	-3.33239104	-3.63141134
C	-1.94554821	-0.37095804	-2.97644389
Si	2.55397392	-0.41901434	-7.03199858
Si	-0.44162042	-0.34576828	-7.49270583

C	3.72324957	-0.52057610	-5.53166779
C	2.99946769	1.19173635	-7.94366330
C	3.08798134	-1.84072633	-8.16753822
C	-0.16061764	-0.77037778	-9.32012174
C	-1.11636222	1.44685798	-7.45920981
C	-1.88554718	-1.42396160	-6.91821004
H	1.47969704	-2.53460670	0.73657212
H	1.88747745	-4.26215904	0.60305700
H	0.18817927	-3.73502067	0.52474486
H	3.47795184	-1.99569659	-1.60573035
H	3.31700807	-2.85142969	-3.15195169
H	3.82390336	-3.73599016	-1.69630741
H	-0.02030341	-5.40621002	-1.98090104
H	1.71716430	-5.78554138	-2.04424715
H	0.91299569	-5.01569624	-3.44585028
H	-2.07800974	-3.53546138	-0.48134179
H	-3.33010156	-2.33024260	-0.85226675
H	-1.87496230	-1.84995848	0.06547518
H	-1.71553067	-4.35163855	-3.40407998
H	-1.75958577	-3.08889152	-4.65999992
H	-3.16722799	-3.33884011	-3.61206122
H	-1.70191963	0.38941039	-2.21835319
H	-3.03093377	-0.35196885	-3.16557764
H	-1.43054088	-0.09578521	-3.91457430
H	3.45426877	0.20245617	-4.74452817
H	4.76569022	-0.32683349	-5.82946277
H	3.70242543	-1.52887185	-5.08370444
H	2.81386887	2.06114344	-7.29264149
H	2.38588120	1.31398234	-8.85069428
H	4.05766049	1.20817563	-8.24996948
H	2.94795861	-2.79840352	-7.64378432
H	4.15324512	-1.74904420	-8.43352187
H	2.50611659	-1.86898915	-9.10056835
H	-0.32547290	2.16984372	-7.72450677
H	-1.51518112	1.72168312	-6.46595260
H	-1.94365638	1.58622100	-8.17215602
H	0.65019708	-0.17312121	-9.76568233
H	-1.07527699	-0.59032784	-9.90643981
H	0.10597919	-1.83307679	-9.43404577
H	-1.62590756	-2.49333728	-6.96339198
H	-2.77022737	-1.26816203	-7.55579573
H	-2.17515092	-1.19302301	-5.88119740
O	1.95717254	-3.58016874	-5.35999690
C	0.89693501	-4.11691181	-6.15667075

C	3.07780694	-4.46117183	-5.34312710
C	1.28749091	-5.56635251	-6.42928404
C	2.81436903	-5.47849380	-6.44969261
H	3.16213589	-5.09004994	-7.41863392
H	3.31183671	-6.43899012	-6.26372020
H	3.99272333	-3.87002582	-5.50127922
H	3.13818363	-4.94743723	-4.35434862
H	0.95411525	-6.21210098	-5.60285787
H	0.85630687	-5.94893927	-7.36301796
H	-0.04499234	-4.02194278	-5.59557946
H	0.81754627	-3.52326269	-7.08383338
O	-0.66364076	2.94898626	-4.05668096
C	-2.07755139	3.01956686	-3.87429459
H	-2.50802666	2.07221364	-4.22625466
H	-2.48478253	3.84018974	-4.48691327
C	-2.31592647	3.25594085	-2.36909181
H	-2.99833678	2.51016185	-1.94193233
H	-2.75392768	4.24956199	-2.20026803
C	-0.90898020	3.17067963	-1.75902313
H	-0.68138364	2.14190840	-1.44353725
H	-0.77463324	3.83369078	-0.89444218
C	-0.02669384	3.55043742	-2.93902267
H	0.99669547	3.15666808	-2.88136352
H	0.01198745	4.64928303	-3.07270858
C	3.37597407	3.14272293	-4.56933148
O	2.11558712	3.12445457	-5.23456241
C	1.83393378	4.38909500	-5.83453825
C	3.09109105	5.23258777	-5.62402532
C	3.67398577	4.62023841	-4.34907388
H	3.28255276	2.55300549	-3.64570864
H	4.13736950	2.66847866	-5.21340331
H	1.59054554	4.23674441	-6.89662226
H	0.95161388	4.82099506	-5.33394788
H	3.78905303	5.08941214	-6.46222124
H	2.87104582	6.30427553	-5.53975009
H	4.74331991	4.82456783	-4.21165458
H	3.13242561	4.98838342	-3.46389177

Table S98. Atomic coordinates and single point energies for **82**.



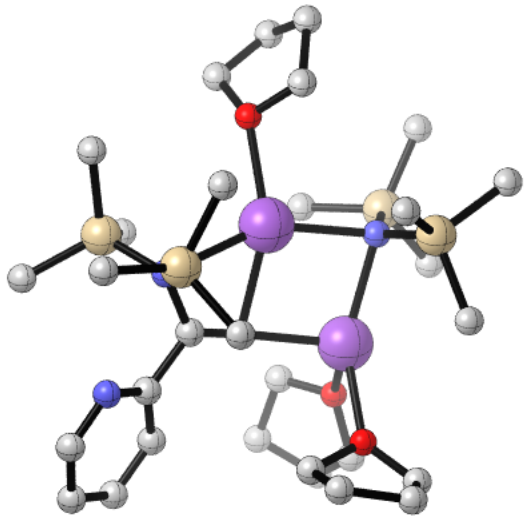
G = –2873.877325
G_{SP} = –2875.96409

N	-3.90440300	-0.85232700	-0.29209600
C	-5.23056800	-0.73044000	-0.23271500
C	-3.17459800	-0.44175600	0.74646900
C	-5.90450700	-0.21757100	0.87256800
C	-3.76217400	0.09770900	1.90171100
C	-5.14489400	0.19915300	1.96834900
H	-5.78927600	-1.06647600	-1.11264800
H	-6.99281000	-0.15464500	0.87567700
H	-5.63129400	0.59645900	2.86151200
H	-3.10775900	0.41600300	2.71383100
C	-1.66256800	-0.49681700	0.64622200
N	-0.92106400	0.36220100	1.15435600
Na	0.05807200	2.27984700	0.50501800
Na	1.12072800	-0.61134900	0.43712000
N	-1.17075700	-1.67380300	-0.14287800
N	2.24254800	1.45924200	0.22467500
Si	-1.18226200	-3.18185100	0.76743000
Si	-1.18752200	-1.52855300	-1.90201500
C	-2.90360600	-3.60320300	1.40324600
C	-0.01796800	-2.97760000	2.23687100
C	-0.58612000	-4.61490700	-0.30059300
C	-2.56225600	-2.44628600	-2.80154900
C	0.44282000	-2.19530500	-2.59768100
C	-1.28062100	0.31626400	-2.27913000
Si	2.80925800	1.69178200	1.81374500
Si	2.73975100	2.10775700	-1.26666500

C	2.31956900	0.20602400	2.89692600
C	1.96761100	3.18970200	2.65061000
C	4.67489000	1.95211400	2.02317900
C	1.52167300	3.45452900	-1.85981500
C	2.73078900	0.79155900	-2.63416200
C	4.45492300	2.91460000	-1.28727500
H	-3.26322600	-2.86117100	2.13155600
H	-2.90167200	-4.58945600	1.89287900
H	-3.62058000	-3.62622600	0.56845400
H	-0.30647400	-2.09394400	2.82749000
H	1.02858500	-2.84178500	1.91590000
H	-0.05078000	-3.85590500	2.89950800
H	-1.21673400	-4.76583600	-1.18911600
H	-0.62903600	-5.53841800	0.29783700
H	0.45113400	-4.47878000	-0.63461300
H	-2.61722500	-3.49927000	-2.48630800
H	-2.37697200	-2.43175400	-3.88709000
H	-3.53133100	-1.97781400	-2.59037300
H	0.45718800	-3.29567000	-2.59365800
H	1.32407000	-1.83525400	-2.04220800
H	0.56028700	-1.86866200	-3.64337100
H	-2.20368100	0.73909200	-1.85420900
H	-1.27183300	0.49715800	-3.36493400
H	-0.42054800	0.84747500	-1.83887500
H	1.22094200	0.10504100	2.92121800
H	2.66022200	0.34317900	3.93470700
H	2.74820400	-0.74411100	2.53573200
H	0.89358400	3.00832900	2.83580100
H	2.06390300	4.09378900	2.02630800
H	2.41357700	3.41489100	3.63186600
H	5.25234200	1.14348000	1.54868900
H	4.93833000	1.97315100	3.09248400
H	5.00372300	2.90135100	1.57518500
H	3.08213700	1.19987500	-3.59471300
H	1.71377100	0.39893100	-2.79240000
H	3.37745400	-0.06257900	-2.37386400
H	0.51642300	3.03753700	-2.04461600
H	1.84921900	3.91644700	-2.80431800
H	1.42626300	4.26188100	-1.11324800
H	4.48867700	3.79187800	-0.62207900
H	4.71417100	3.25214800	-2.30309000
H	5.23521700	2.21347600	-0.95231000
O	2.89291000	-2.04691100	0.17051900
C	4.18319900	-1.42525400	0.19811700

C	3.01712900	-3.42536400	-0.18870500
C	5.05209600	-2.30599500	-0.68504300
C	4.51630300	-3.69327600	-0.33020100
H	4.94038900	-4.02628600	0.62862000
H	4.73365100	-4.45954600	-1.08496800
H	2.53879600	-4.04803200	0.58245500
H	2.48855700	-3.58418000	-1.14231400
H	4.86631500	-2.07871100	-1.74607100
H	6.12403800	-2.18333900	-0.48499500
H	4.06450900	-0.38848700	-0.14310300
H	4.56176100	-1.41042500	1.23582700
O	-1.71389600	3.50034800	-0.13718100
C	-2.81943500	3.24214800	0.73439600
H	-3.02236200	4.13948600	1.34537100
H	-2.54248400	2.40052900	1.38520700
C	-3.97938000	2.93704400	-0.19943300
H	-4.95921400	3.07541300	0.27587400
H	-3.91197700	1.89458900	-0.54975500
C	-3.70570500	3.91804400	-1.34151600
H	-4.05962300	4.92340700	-1.06853400
H	-4.18284300	3.63437800	-2.28825700
C	-2.17776100	3.89353200	-1.43211000
H	-1.74252700	4.86926100	-1.69262300
H	-1.83056500	3.15019000	-2.16730300

Table S99. Atomic coordinates and single point energies for **81**.



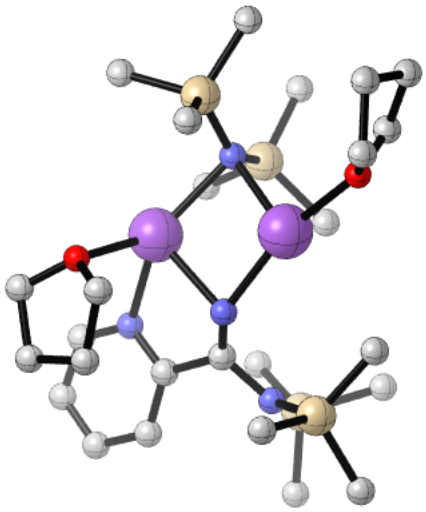
G = –3105.95436
G_{SP} = –3108.304119

N	3.79088400	-1.97902200	0.35196900
C	5.12152600	-2.01549200	0.30745500
C	3.14885600	-1.03693400	-0.34288800
C	5.88868200	-1.13023400	-0.44621700
C	3.83662300	-0.08882900	-1.11599300
C	5.22249800	-0.14410200	-1.17626900
H	5.60643000	-2.79755700	0.90116900
H	6.97559300	-1.21370100	-0.45868300
H	5.78291900	0.57002700	-1.78316600
H	3.24716800	0.66566700	-1.63796400
C	1.63290800	-0.95295000	-0.26387200
N	0.99874900	0.08886100	-0.51086700
Na	-0.05903800	2.03711700	-0.04267900
Na	-1.12931600	-0.84822600	-0.08086100
N	0.99577900	-2.23707900	0.14889500
N	-2.27151800	1.16136300	0.38491200
Si	0.90354700	-3.45395600	-1.12128400
Si	1.01186200	-2.62081800	1.87335300
C	2.55252900	-4.28380400	-1.49546100
C	0.32087300	-2.58519700	-2.69016000
C	-0.33465500	-4.78000200	-0.61467500
C	2.07493200	-4.10979800	2.31257900
C	-0.75590100	-2.99047500	2.43656100
C	1.59174800	-1.08337400	2.79295600
Si	-3.08858800	1.52661300	-1.06659300

Si	-2.65184300	1.70364400	1.95526300
C	-2.37020900	0.43207400	-2.45062700
C	-2.86119600	3.32340100	-1.64384200
C	-4.96626300	1.22722000	-1.06675900
C	-4.42236300	2.34468300	2.18676900
C	-1.49778000	3.12749800	2.48467000
C	-2.39041600	0.35721100	3.26596600
H	3.27472200	-3.56755600	-1.91479100
H	2.41371500	-5.10005300	-2.22193700
H	2.99240100	-4.70071900	-0.57731000
H	1.07726500	-1.85619800	-3.02009900
H	-0.61785700	-2.02838800	-2.54177700
H	0.16419600	-3.30950700	-3.50445000
H	0.02810000	-5.37870600	0.23451500
H	-0.50823000	-5.46857000	-1.45636200
H	-1.29206300	-4.32166200	-0.32928800
H	1.72102200	-5.02451200	1.81289800
H	2.05096000	-4.29277100	3.39801300
H	3.11096300	-3.92102500	2.00064100
H	-1.17992000	-3.85686900	1.90832700
H	-1.42436100	-2.13065900	2.27113900
H	-0.77411200	-3.20568400	3.51678200
H	2.64479000	-0.86466300	2.56082300
H	1.49162800	-1.22238900	3.88031700
H	0.98628800	-0.21096200	2.49765800
H	-1.26846000	0.48888200	-2.46919900
H	-2.73924000	0.72810900	-3.44487500
H	-2.64808200	-0.62400700	-2.29848200
H	-1.79903200	3.55296700	-1.83060400
H	-3.23017800	4.02132400	-0.87425200
H	-3.41896700	3.52421900	-2.57263600
H	-5.22548400	0.26185400	-0.60483700
H	-5.36070100	1.23026000	-2.09600600
H	-5.49305600	2.01262700	-0.50445800
H	-1.54038700	3.95105500	1.75091700
H	-0.45365600	2.77621500	2.54934300
H	-1.76935100	3.53910000	3.46948600
H	-4.62850200	3.20002200	1.52336100
H	-4.58736200	2.67565800	3.22419100
H	-5.16195500	1.56091300	1.95919700
H	-3.05524700	-0.50593100	3.10247400
H	-2.59177200	0.74552000	4.27692000
H	-1.35159800	-0.01076700	3.25405100
O	-2.83063700	-2.38073600	-0.36465400

C	-3.88302400	-2.09363500	0.57033400
C	-3.36420800	-3.06659600	-1.49168500
C	-5.19227800	-2.50537100	-0.11728800
C	-4.79618400	-2.56563100	-1.59463000
H	-4.80754000	-1.55880300	-2.03960600
H	-5.43961000	-3.22271500	-2.19360500
H	-2.73697600	-2.83835800	-2.36485900
H	-3.33531100	-4.15794000	-1.31963800
H	-5.51404400	-3.49874200	0.22766300
H	-6.00747600	-1.79805100	0.08367600
H	-3.70287200	-2.65425100	1.50055900
H	-3.83892500	-1.01469100	0.79016400
O	1.62839000	3.10588300	1.08540800
C	1.77372100	4.30221800	1.82809400
H	0.79102500	4.78426700	1.90438700
H	2.46566400	4.97986100	1.29358100
C	2.36371300	3.86740600	3.17889000
H	1.56752900	3.75486500	3.92646400
H	3.07901200	4.60693200	3.56130400
C	3.02150400	2.50301500	2.86249700
H	2.52516700	1.69324800	3.41347400
H	4.08893200	2.47401400	3.11575000
C	2.79050300	2.33289100	1.35658600
H	2.59716000	1.30516200	1.02448700
H	3.63954700	2.73954900	0.77456500
C	0.85311100	2.31963900	-3.05727800
O	0.63497400	3.14321900	-1.90720800
C	1.53903700	4.24016000	-1.89157000
C	2.02627300	4.36906300	-3.32908000
C	2.08720600	2.89953600	-3.74836400
H	0.98696900	1.28091400	-2.71725800
H	-0.03948800	2.38005300	-3.70217800
H	1.00629300	5.12734300	-1.51983300
H	2.37305900	4.01908900	-1.20228400
H	1.28391800	4.91022300	-3.93492200
H	2.98811600	4.89187900	-3.40924400
H	2.07104700	2.74875200	-4.83521200
H	3.00274900	2.43393300	-3.35280200

Table S100. Atomic coordinates and single point energies for **83**.



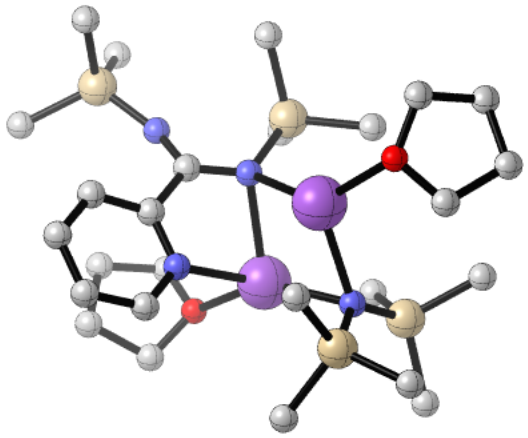
G = –2873.886683
G_{SP} = –2875.973666

N	-2.06076800	-2.00567000	0.85804300
C	-2.78056800	-3.02676100	1.32178700
C	-2.68727100	-0.99865900	0.23221900
C	-4.15949400	-3.13587100	1.15213800
C	-4.07078300	-1.03429700	0.00056000
C	-4.81167200	-2.12042200	0.45352300
H	-2.23009500	-3.80522400	1.86052600
H	-4.69798900	-3.99528200	1.55092200
H	-5.88741400	-2.17127100	0.27466800
H	-4.53430100	-0.19951200	-0.52534600
C	-1.83128100	0.16524800	-0.26038600
N	-0.68255500	0.00486100	-0.72434900
Na	0.29267100	-1.85917600	0.26985900
Na	1.38340500	0.88545700	-0.62037800
N	-2.54871900	1.43037000	-0.21358300
N	2.26090100	-0.66392700	0.87853000
Si	-2.13819900	2.47563000	-1.57611400
Si	-3.19268200	2.04744700	1.31337300
C	-2.16754000	1.49074700	-3.17838200
C	-0.46746900	3.35361400	-1.38522500
C	-3.48844800	3.78935900	-1.72918000
C	-5.04857500	2.36236100	1.21436100
C	-2.32770900	3.66110600	1.77624100
C	-2.85869900	0.82230900	2.70571300
Si	3.56907200	-1.59604100	0.32643000

Si	1.84549100	-0.06384300	2.41550000
C	5.29361000	-1.00440900	0.86159200
C	3.54001800	-1.60358000	-1.57549400
C	3.46239700	-3.41804000	0.85917500
C	3.30118100	0.27250600	3.58196600
C	0.66708700	-1.22802300	3.35139600
C	0.89699900	1.57671000	2.20111200
H	-1.32359400	0.78941600	-3.22392600
H	-2.11697700	2.16896200	-4.04445800
H	-3.10173900	0.91225200	-3.25468000
H	0.30402200	2.86236100	-1.99823200
H	-0.14224800	3.33819900	-0.33300000
H	-0.51743100	4.40620100	-1.70374200
H	-4.46351600	3.31489200	-1.91891400
H	-3.26143300	4.44269200	-2.58626200
H	-3.59098800	4.43184600	-0.84284600
H	-5.29939000	3.07242100	0.41331400
H	-5.41286300	2.78114900	2.16543600
H	-5.59720800	1.42680900	1.02828600
H	-2.37564400	4.42340400	0.98528200
H	-1.26693200	3.46813100	1.99721800
H	-2.78982800	4.08735200	2.68046600
H	-3.53325200	-0.04599200	2.67918700
H	-3.00475000	1.33574800	3.66914300
H	-1.82257900	0.45109700	2.67541800
H	5.46667500	0.05158700	0.60191600
H	6.08042000	-1.60433800	0.37683700
H	5.42104200	-1.09993900	1.95070200
H	3.53217200	-0.57267700	-1.96799200
H	2.63088300	-2.11070300	-1.93958200
H	4.40681500	-2.12330600	-2.01262800
H	3.47589200	-3.49917000	1.95813700
H	4.29733100	-4.01873900	0.46528400
H	2.52671800	-3.87939800	0.49995800
H	1.14714300	-2.20936000	3.50184800
H	-0.27537900	-1.39112900	2.80041900
H	0.39630700	-0.83093200	4.34251800
H	3.81412600	-0.66687300	3.84328300
H	2.96089800	0.74146600	4.51852800
H	4.04547100	0.93915400	3.11814400
H	1.54211800	2.36752600	1.77918500
H	0.50544300	1.95529000	3.15855200
H	0.03467700	1.43379100	1.52475400
O	3.18159000	2.11841600	-1.21418700

C	3.95865200	2.45826900	-0.05611200
C	3.99983300	2.14796600	-2.37717700
C	5.40513900	2.60790900	-0.54307200
C	5.39659300	1.83376300	-1.86317900
H	5.48865700	0.75239800	-1.67741400
H	6.19001800	2.14140600	-2.55618400
H	3.60965400	1.41215300	-3.09443800
H	3.95900200	3.14880600	-2.84257200
H	5.64361100	3.66566300	-0.72666000
H	6.13016400	2.21845000	0.18339400
H	3.56531200	3.38714200	0.38422800
H	3.84105700	1.63895300	0.67132000
O	-0.06069600	-3.25994300	-1.49490300
C	-1.01345400	-4.30773700	-1.51571900
H	-1.17369000	-4.64765700	-0.48345200
H	-0.61421300	-5.15327100	-2.10418700
C	-2.26785600	-3.71555800	-2.17951700
H	-3.00652900	-3.41272500	-1.42526900
H	-2.74758300	-4.44806400	-2.84196100
C	-1.72858400	-2.48448100	-2.94269800
H	-2.11189000	-1.55560900	-2.50028300
H	-1.98679900	-2.49432400	-4.00960400
C	-0.21608400	-2.55565100	-2.71983300
H	0.24517200	-1.56682000	-2.60439700
H	0.29178100	-3.11566600	-3.52639000

Table S101. Atomic coordinates and single point energies for **84**.



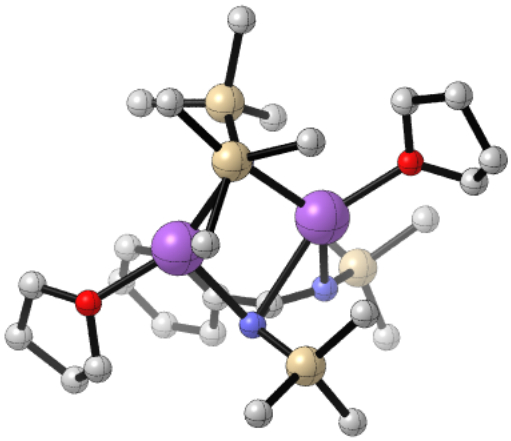
G = –2873.903188
G_{SP} = –2875.990727

N	-0.92460300	-1.57129400	1.25050400
C	-0.91006000	-2.60896200	2.09093900
C	-1.92120400	-0.67974700	1.33167900
C	-1.87918500	-2.81429500	3.06855100
C	-2.93292800	-0.80586700	2.29315900
C	-2.90975900	-1.88121600	3.17280500
H	-0.07233500	-3.30571900	1.98914700
H	-1.81640500	-3.67614200	3.73243100
H	-3.68350600	-1.98865600	3.93499700
H	-3.71233400	-0.04829600	2.34724500
C	-1.93582200	0.50509900	0.35920900
N	-0.72922400	0.88743700	-0.09176100
Na	0.22382500	-1.18371300	-0.84474000
Na	1.42911100	0.78026000	0.83402500
N	-3.06631100	1.04265600	0.04255700
N	2.50763300	-0.93640300	-0.32987600
Si	-0.74694800	2.34218700	-1.07714200
Si	-4.69434400	1.48934700	0.21309600
C	-1.50203300	2.09169000	-2.78620100
C	1.08515400	2.80946000	-1.27262200
C	-1.55051600	3.83434900	-0.24393300
C	-5.25828800	2.36450100	-1.35900300
C	-4.85578000	2.68072600	1.67191800
C	-5.95622500	0.09300700	0.48103400
Si	3.17383900	-0.79581500	-1.89622000
Si	3.04965800	-1.95458700	0.92669100
C	4.41058000	0.63727500	-2.05358100

C	1.77105400	-0.49858300	-3.15579200
C	4.06539900	-2.34085900	-2.54176400
C	4.93092300	-2.09618500	1.13921700
C	2.41930300	-3.73969100	0.73911600
C	2.41680500	-1.28440300	2.59732000
H	-1.02532500	1.26372300	-3.33324300
H	-1.39834500	3.00261900	-3.39605400
H	-2.57365200	1.87010000	-2.67695900
H	1.71437600	1.97033300	-1.60813900
H	1.49035100	3.17695200	-0.31513400
H	1.20719300	3.62439700	-2.00265400
H	-2.63866900	3.83850800	-0.38993700
H	-1.13855900	4.77208700	-0.64887800
H	-1.35711600	3.81547800	0.84060300
H	-4.64166200	3.25163300	-1.56753600
H	-6.30968700	2.68344100	-1.28721200
H	-5.17000500	1.68619000	-2.22268400
H	-4.15735500	3.52304900	1.55985300
H	-4.63027900	2.18729700	2.63019900
H	-5.87771100	3.08560400	1.73527900
H	-6.10532300	-0.49044400	-0.43981700
H	-6.92832800	0.53807300	0.74780600
H	-5.67912300	-0.61020000	1.28085600
H	3.97478300	1.59001400	-1.71029300
H	4.75296900	0.77398600	-3.09111900
H	5.29781300	0.42855100	-1.43254500
H	1.09722400	0.32495800	-2.86766000
H	1.16176300	-1.41063600	-3.28527900
H	2.17407300	-0.24867700	-4.14917000
H	4.95540400	-2.58631800	-1.94304400
H	4.39441300	-2.19638300	-3.58304600
H	3.39309800	-3.21324400	-2.51969700
H	2.97786800	-4.24381100	-0.06548800
H	1.35559500	-3.75735700	0.44939700
H	2.53792500	-4.33797000	1.65649600
H	5.40480800	-2.54993900	0.25593700
H	5.17658100	-2.72693600	2.00845000
H	5.39578800	-1.11099200	1.29919600
H	2.88018100	-0.31141800	2.83525600
H	2.67629300	-1.96845400	3.42010100
H	1.32166500	-1.15961200	2.61703100
O	2.98317700	2.17559800	1.68608600
C	4.31064100	1.69642900	1.44234500
C	3.04660200	3.57966600	1.88103000

C	5.12427200	2.90632300	0.94042100
C	4.08829300	4.03909100	0.86937800
H	3.63051100	4.08404400	-0.12980500
H	4.50833600	5.02560800	1.10304000
H	2.04194500	3.99581700	1.72309900
H	3.36322600	3.80364200	2.91602900
H	5.92437500	3.15424900	1.65109200
H	5.58973200	2.70859700	-0.03347200
H	4.72690300	1.28763300	2.37803600
H	4.23170000	0.88289500	0.70671000
O	-1.46506300	-2.30679300	-1.78091500
C	-1.84203900	-3.59924000	-1.33889300
H	-1.05450200	-3.97716200	-0.67154100
H	-1.92168100	-4.27622600	-2.20835200
C	-3.20001500	-3.41032000	-0.65491400
H	-3.06883000	-3.25295200	0.42493800
H	-3.84499000	-4.28799000	-0.79005700
C	-3.76616900	-2.13645000	-1.32115200
H	-3.96886000	-1.36470900	-0.56985100
H	-4.69637800	-2.32562000	-1.87308000
C	-2.64380800	-1.66906100	-2.25914700
H	-2.48110100	-0.58245400	-2.22977900
H	-2.82655800	-1.98266200	-3.30185600

Table S102. Atomic coordinates and single point energies for **85**.



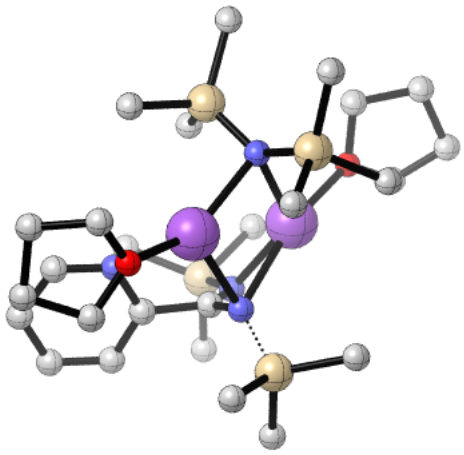
G = –2873.909439
G_{SP} = –2875.996627

N	2.33887300	0.10715100	-1.18564500
C	3.35629400	-0.04284100	-2.03668500
C	2.27124700	1.23105200	-0.46304300
C	4.38171500	0.88851400	-2.17567500
C	3.25542900	2.22459300	-0.53471800
C	4.33406000	2.04118500	-1.39096400
H	3.35579700	-0.95612800	-2.64076400
H	5.19462900	0.71009200	-2.87938800
H	5.12387900	2.79154100	-1.45699000
H	3.15962200	3.11870600	0.08286000
C	1.08238600	1.38225400	0.46795700
N	1.04902400	0.47495400	1.43913200
Na	1.06885000	-1.53103100	0.18823800
Na	-1.37061100	0.48372300	0.11293600
N	0.18217200	2.30522000	0.22814900
N	-1.14990100	-1.75410100	-0.56358100
Si	0.23614900	0.81412900	2.94615600
Si	0.04481000	3.66656700	-0.84028000
C	0.57591900	2.57203500	3.52991100
C	0.93076000	-0.37218800	4.23587000
C	-1.65489500	0.60174500	2.87663000
C	0.75726500	5.20197600	-0.00261500
C	-1.80215700	3.94694100	-1.08465400
C	0.83398200	3.51002000	-2.55316900
Si	-1.76367500	-3.00369100	0.42387600
Si	-1.11622000	-1.67122800	-2.26915000
C	-3.54392400	-2.69045400	1.01381800

C	-0.68596100	-3.15104500	1.98541900
C	-1.77035900	-4.73331700	-0.35496200
C	-2.57916800	-2.46163700	-3.18445200
C	0.44491300	-2.47698000	-2.99765700
C	-1.05148400	0.16085400	-2.77125900
H	1.66029400	2.74360400	3.61165300
H	0.12627700	2.75668700	4.51765800
H	0.16701400	3.29532500	2.81057300
H	1.98896000	-0.13061700	4.42211300
H	0.87682900	-1.42390300	3.91842100
H	0.39323300	-0.27706600	5.19184200
H	-2.10868500	1.42240700	2.29716900
H	-2.07640400	0.65383100	3.89234800
H	-1.97243000	-0.36319000	2.44737600
H	0.29592400	5.34975200	0.98533400
H	0.56443200	6.10116500	-0.60818600
H	1.84542100	5.12536300	0.14360700
H	-2.27766200	4.15757600	-0.11416400
H	-2.28613000	3.05376800	-1.51050100
H	-1.99586700	4.79862900	-1.75429300
H	1.93230600	3.48928000	-2.51960200
H	0.53293500	4.37887500	-3.16039900
H	0.49029500	2.60430800	-3.07447500
H	-3.66355300	-1.67122800	1.41879600
H	-3.84745500	-3.40547300	1.79431700
H	-4.24407800	-2.80105300	0.16929700
H	-0.58444800	-2.17778100	2.49058000
H	0.32864100	-3.51846400	1.75006200
H	-1.11774800	-3.85546300	2.71289300
H	-2.47748900	-4.80032400	-1.19533800
H	-2.06081200	-5.49407300	0.38690100
H	-0.76980200	-4.99694700	-0.73325300
H	0.48226900	-3.54732400	-2.73847100
H	1.34477500	-1.99017900	-2.58684600
H	0.48984700	-2.39059000	-4.09461500
H	-2.55309700	-3.55838800	-3.09881800
H	-2.54060500	-2.21214000	-4.25672900
H	-3.54982900	-2.11798100	-2.79495700
H	-1.96065400	0.70772800	-2.46600000
H	-0.94027800	0.29369800	-3.85849100
H	-0.18056800	0.64039400	-2.29254000
O	-3.49934500	1.09597000	-0.21800300
C	-4.34023300	0.16120900	-0.89306100
C	-4.33535300	2.00476600	0.47724000

C	-5.64995300	0.09592000	-0.07836500
C	-5.42460500	1.11118600	1.05639200
H	-5.03785100	0.60893300	1.95562900
H	-6.33287800	1.66215600	1.33172700
H	-3.72819200	2.53172100	1.22502600
H	-4.74943900	2.74958900	-0.22739800
H	-6.50697100	0.38498200	-0.70142700
H	-5.84011100	-0.91344000	0.30762600
H	-4.52183700	0.51267000	-1.92293700
H	-3.79435700	-0.79125900	-0.93513500
O	3.03116700	-2.46800800	0.77056700
C	3.99288700	-2.96618800	-0.15148400
H	3.56692300	-2.87325600	-1.16182400
H	4.17532300	-4.03535100	0.04318200
C	5.27194300	-2.12594900	0.04897200
H	5.62612800	-1.67890300	-0.88937500
H	6.08205100	-2.75309000	0.44639600
C	4.85180400	-1.06321900	1.07544700
H	4.47726600	-0.15848600	0.57410400
H	5.66779700	-0.77062300	1.74864500
C	3.70239400	-1.74923000	1.80087600
H	2.98040000	-1.05062900	2.24402900
H	4.06923900	-2.45335800	2.56990200

Table S103. Atomic coordinates and single point energies for **TS-18**.



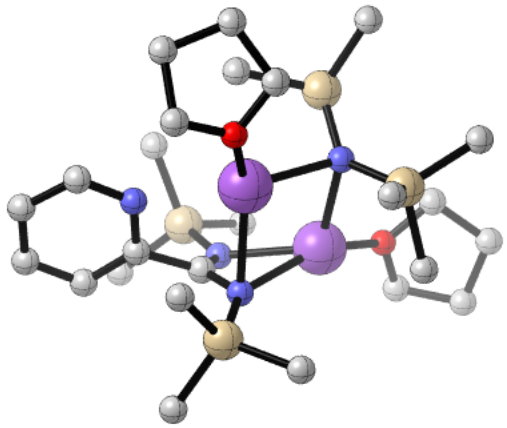
G = –2873.900477
G_{SP} = –2875.989278

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.33280190
C	1.17540561	0.00000000	-0.64157754
C	1.16445323	0.05234105	2.09635419
C	2.39811543	0.06232459	0.03731608
C	2.38780291	0.10453053	1.42737442
H	-0.98166565	-0.03318043	1.81769750
H	1.10954953	0.05771914	3.18495564
H	3.32346731	0.16254931	1.98638893
H	3.32985407	0.07068343	-0.53010132
C	1.08627382	-0.06977498	-2.15546693
N	0.54865269	1.00995502	-2.74005111
Na	-1.51812992	1.15065923	-1.62490025
Na	-0.60249600	-0.71745937	-4.01016442
N	1.38773308	-1.17703939	-2.76122167
N	-2.72694161	-0.19119376	-3.13121609
Si	1.32976934	2.40643241	-3.35846826
Si	2.04107825	-2.70826662	-2.23612766
C	3.19705257	2.12715614	-3.40102616
C	0.97910419	3.92853642	-2.28822367
C	0.73177237	2.80885147	-5.10292180
C	3.92421501	-2.62010973	-2.30077114
C	1.45706590	-3.96829104	-3.50623045
C	1.52610282	-3.29895255	-0.51580746
Si	-3.40035751	0.91809078	-4.22401340
Si	-3.34767755	-1.38318214	-2.09288160

C	-2.52337590	0.82125100	-5.91267179
C	-3.14353379	2.70568355	-3.61217643
C	-5.25258546	0.72051941	-4.56805663
C	-4.95308879	-2.23668015	-2.63342412
C	-3.71232414	-0.68386438	-0.35219949
C	-2.01934953	-2.71319039	-1.85533519
H	3.59510901	2.02817964	-2.37849511
H	3.72798346	2.95808066	-3.88972912
H	3.42898509	1.19787611	-3.94407425
H	1.43678173	3.80667394	-1.29362897
H	-0.10562133	4.06777086	-2.14611579
H	1.38272985	4.84921940	-2.73771379
H	0.94770541	1.97483668	-5.78947158
H	1.23101589	3.70899908	-5.49426996
H	-0.35367670	2.99259966	-5.12321558
H	4.25479977	-2.22112029	-3.27134488
H	4.36857021	-3.61881698	-2.16942601
H	4.32712562	-1.96807811	-1.51112519
H	1.87181164	-3.71712196	-4.49473184
H	0.35903355	-3.95359550	-3.58756831
H	1.77525900	-4.98937377	-3.24716109
H	1.89836121	-2.64435749	0.28590481
H	1.94023233	-4.30593932	-0.34659959
H	0.43237131	-3.36707931	-0.42473297
H	-1.44197941	1.02089981	-5.82404930
H	-2.92399850	1.56144944	-6.62294974
H	-2.64737906	-0.17753913	-6.36157656
H	-2.07248210	2.93249444	-3.46681561
H	-3.65739339	2.86544159	-2.64883923
H	-3.53416785	3.45128875	-4.32207889
H	-5.47584712	-0.28062493	-4.96943725
H	-5.60426308	1.46662417	-5.29777201
H	-5.83996858	0.84624851	-3.64457861
H	-4.47660286	0.10879435	-0.41645949
H	-2.80243422	-0.25778384	0.10695942
H	-4.08846109	-1.45782882	0.33523637
H	-5.78859396	-1.52204541	-2.68227065
H	-5.22573387	-3.02700079	-1.91608250
H	-4.85671869	-2.70480087	-3.62537496
H	-1.78296058	-3.20770201	-2.81220682
H	-2.29845603	-3.49156431	-1.12825536
H	-1.09956219	-2.22364261	-1.49363464
O	-1.07750665	-2.38602808	-5.44069153
C	-2.41320960	-2.85603337	-5.58303601

C	-0.34263916	-2.87637126	-6.54743490
C	-2.67372288	-2.93972371	-7.10268334
C	-1.28869280	-2.67767708	-7.72932638
H	-1.21675072	-1.64067058	-8.08629779
H	-1.06176328	-3.34538424	-8.57012053
H	0.59785542	-2.31365941	-6.61472044
H	-0.10498687	-3.94524616	-6.39421195
H	-3.06059934	-3.93024748	-7.37562878
H	-3.41163326	-2.19613017	-7.43074185
H	-2.50065946	-3.84923193	-5.10897199
H	-3.06428894	-2.15197848	-5.04711399
O	-1.82030539	2.76455419	-0.09080032
C	-3.04517755	3.05709630	0.55890769
H	-3.83311527	2.44376201	0.10257299
H	-3.29703239	4.12469130	0.42249422
C	-2.76431019	2.73137672	2.02223514
H	-2.87804876	1.64866898	2.17771091
H	-3.44432630	3.24712122	2.71184833
C	-1.29245173	3.16100560	2.18510002
H	-0.71654766	2.43163402	2.76930936
H	-1.21146574	4.12983336	2.69550433
C	-0.77547173	3.26722902	0.73345779
H	0.12552563	2.67007218	0.53471019
H	-0.56644878	4.31387211	0.45681170

Table S104. Atomic coordinates and single point energies for **86**.



G = –2873.90509
G_{SP} = –2875.993758

N	2.76671400	0.75636200	-0.46449200
C	3.99558100	0.78748800	-0.98049700
C	2.27959100	1.86937200	0.10254700
C	4.81960300	1.90891000	-0.92128900
C	3.03388200	3.04158700	0.21304800
C	4.32810900	3.05453300	-0.29676300
H	4.34344300	-0.12977200	-1.46573600
H	5.82040200	1.87917600	-1.35121100
H	4.94545400	3.95106000	-0.21664000
H	2.59648800	3.91890500	0.69051800
C	0.84097700	1.76023900	0.57842900
N	0.58888800	0.96227900	1.61558000
Na	1.05975900	-0.95675100	0.13628700
Na	-1.57693300	0.68914800	0.59401100
N	-0.09230400	2.32789700	-0.13897800
N	-1.18046800	-1.48581400	-0.30227300
Si	1.58071900	0.62631900	2.99727000
Si	-0.11930500	3.34890200	-1.54212700
C	2.20261700	2.21852700	3.79881000
C	3.09863800	-0.45401500	2.62797500
C	0.52557500	-0.31540100	4.23680100
C	0.74034900	5.01595000	-1.28298300
C	-1.93654400	3.72279700	-1.86580400
C	0.64286300	2.53247800	-3.06421900
Si	-1.89219000	-2.41364800	0.93246400
Si	-1.13721900	-1.59260000	-1.99923800
C	-2.63265300	-1.26889300	2.27060300

C	-0.65533600	-3.52104500	1.86478600
C	-3.30043000	-3.56664500	0.39453700
C	-1.60814500	-3.27806100	-2.73626500
C	0.63143300	-1.21820900	-2.61767000
C	-2.23824100	-0.31618900	-2.87184700
H	2.90402000	2.74852500	3.13625100
H	2.72606900	2.00851400	4.74432100
H	1.36072400	2.89363000	4.01428600
H	3.81162900	0.05543400	1.96077500
H	2.81691400	-1.41509700	2.16540600
H	3.62346500	-0.68911500	3.56750000
H	-0.35750700	0.27604100	4.52235700
H	1.09672300	-0.54310100	5.14986200
H	0.17110200	-1.26743100	3.81206700
H	0.50958000	5.42795900	-0.28829800
H	0.38126500	5.73481100	-2.03632800
H	1.83269900	4.94438200	-1.38625000
H	-2.33647000	4.33625800	-1.04285300
H	-2.53103200	2.79743400	-1.90851500
H	-2.07963900	4.27613600	-2.80644800
H	1.68599000	2.23147900	-2.87372800
H	0.64086000	3.22956100	-3.91688600
H	0.07734700	1.63524400	-3.35718200
H	-1.86146800	-0.61749000	2.71623100
H	-3.06440000	-1.85931500	3.09338700
H	-3.43762400	-0.63057700	1.86915700
H	0.31114200	-3.01624100	2.03443300
H	-0.45065100	-4.44156900	1.29613400
H	-1.05245100	-3.82242500	2.84716900
H	-4.09948700	-3.02149200	-0.13351900
H	-3.75178600	-4.06377400	1.26788700
H	-2.92968400	-4.35009400	-0.28414400
H	1.36628600	-1.95034400	-2.24273700
H	0.96648200	-0.21482700	-2.30454000
H	0.67804500	-1.24281700	-3.71768500
H	-1.00918900	-4.10006200	-2.31179500
H	-1.45911500	-3.28045400	-3.82782700
H	-2.66728700	-3.50748700	-2.54246900
H	-3.29598300	-0.61966000	-2.84466300
H	-1.95524200	-0.19374000	-3.92952000
H	-2.15709800	0.66826400	-2.38163400
O	-3.69853200	1.24615100	0.05861000
C	-4.60654000	0.28068800	-0.45018300
C	-4.48644300	2.29622600	0.58855200

C	-5.78911100	0.26690600	0.53726400
C	-5.61307900	1.57854500	1.33749100
H	-5.29855300	1.36268500	2.36777100
H	-6.52950600	2.18034500	1.38398700
H	-3.84549200	2.92476300	1.22036600
H	-4.88144300	2.91420700	-0.23819200
H	-6.74706500	0.23098100	0.00286400
H	-5.74539100	-0.60949200	1.19735900
H	-4.93200400	0.58927900	-1.45878500
H	-4.06591500	-0.67246100	-0.53349800
O	2.31849500	-2.83084000	0.08434100
C	1.76830800	-4.00482500	-0.50262800
H	0.71634600	-3.79249400	-0.73976000
H	1.80261700	-4.82581600	0.23299600
C	2.64802800	-4.31350100	-1.73284800
H	2.10672100	-4.13425200	-2.67102800
H	2.96593100	-5.36413900	-1.72935700
C	3.84742100	-3.35321300	-1.58002400
H	3.74268600	-2.49755600	-2.26323000
H	4.81320900	-3.83398600	-1.78092900
C	3.71713400	-2.87596900	-0.13480500
H	4.12545000	-1.87589600	0.06314300
H	4.18217500	-3.59134200	0.56815500