Content

1 Experimental Details – Materials and General Methods

All used reagents and solvents were purchased from commercial sources. Unless otherwise noted, all manipulations were carried out under a dry nitrogen or argon atmosphere. Solvents were degassed prior to use with four freeze-pump-thaw cycles and were stored in sealed Schlenk ampulla over activated molecular sieve (3 or 4 Å, respectively) under a dry argon atmosphere. Liquid reactants were degassed for at least 10 min with a constant stream of dry argon through the fluid phase and were dried by storage over activated molecular sieve (3 or 4 Å, respectively). Solid reagents were dried and purified if necessary either by the application of vacuum and elevated temperature, or by sublimation under reduced pressure at elevated temperature. N-methylindole and N-methylpyrrole were filtered over silica prior to use.
All reactions on preparative scale were carried out in flame-dried standard laboratory glassware under a dry argon atmosphere using Schlenk line techniques and were permanently magnetically stirred. Syringes, magnetic stirring bars, and needles were dried and/or flushed with argon prior to use. Reaction on the NMR sample scale were done in dry *J. Young* NMR tubes.
Compounds sensitive to ambient conditions were handled and stored in a *Sylatech* glove box filled with dry nitrogen gas. Removal of solvents in *vacuo* was performed using a *Heidolph VV2000* rotary evaporator or a Schlenk line.
Literature-known compounds were synthesized following published procedures, which are cited (see below). Analytical data of known compounds were compared to data of the respective reference and were found to be consistent in all cases. Novel compounds were characterized to the reported structures to the best of our knowledge.
Nuclear magnetic resonance (NMR) spectra were collected with a *Bruker BZH 200/52*, a *Bruker Avance I 200*, a *Bruker Avance II 400*, or a *Bruker Avance III 600* spectrometer at 298 K unless otherwise noted. Measurements were partially carried out by the NMR facility of the Institute of Inorganic Chemistry of Heidelberg University.
Chemical shifts δ are given in parts per million (ppm) relative to the tetramethylsilane resonance. Deuterated dichloromethane and chloroform were used as solvent, and the signal of $CHDCl_2$ or $CHCl_3$ was used for calibration of the spectra (CD_2Cl_2: ^{1}H: 5.32 ppm, ^{13}C: 53.84 ppm, $CDCl_3$: ^{1}H: 7.26 ppm, ^{13}C: 77.16 ppm). ^{1}H and ^{19}F NMR data is reported as follows: chemical shift δ [ppm], multiplicity (s = singlet, br = broad singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sext = sextet, sept = septet, m = multiplet, and combinations; pseudo-multiplicities are reported likewise), scalar spin-spin coupling constant [Hz] as $^{X}J_{AB}$ (if apparent: X = number of chemical bonds between coupled nuclei; A, B = coupled nuclei), integration value. ^{13}C and ^{29}Si spectra were recorded ^{1}H-decoupled if not stated otherwise. ^{13}C and ^{29}Si data is reported as follows: chemical shift δ [ppm], multiplicity (if apparent), scalar spin-spin coupling constant [Hz] as $^{(X)}J_{(AB)}$. NMR spectra were processed and plotted with *MestReNova 14.2*.
High resolution mass spectrometry (HR-MS) was conducted with the electrospray ionization method (ESI) on a *Bruker ApexQe hybrid 9.4 T FT-ICR*, carried out by the Mass Spectrometry Facility of the Institute of Organic Chemistry of the University of Heidelberg. Mass spectrometry data is reported as follows: *m/z* ratio (relative intensity) [assigned fragment] (for HR experiments: calculated exact mass).
Gas chromatography mass spectroscopy (GCMS) experiments were conducted utilizing helium as carrier gas on a *Thermo Fischer Scientific Ultra Trace* gas chromatograph equipped with a *TraceGOLD* TG-1701MS column (14% cyanopropylphenyl, 86% dimethylpolysiloxane, 30 m x 0.25 mm x 0.25 µm) and a *Thermo Fischer Scientific* ISQ Single Quadropole Mass Selective Detector. Unless stated otherwise, the following column program was used: at a constant pressure of 50 kPa the initial temperature of 35 °C was held for 5 min after injection, then increased by 30 K/min to 250 °C, this temperature kept for 10 min before cooling to 150 °C at a rate of 25 K/min. Reported retention times refer to this program.

2 Comparison of pK_a Values

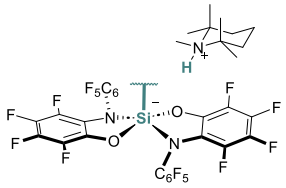
To assess the possibility of pmp to deprotonate the substrates in the absence of a Lewis acid, pK_a values of the respective compounds were compared (listed in **Table S1**). Due to limited data for pmp, related N-methylpiperidine was considered, for which pK_a values in acetonitrile are in good agreement. Further comparison of the respective substrates with the amine reveals a difference of several orders of magnitude, rendering a non-assisted deprotonation highly implausible.

Table S1. Collected pK_a data for substrates, pmp, and related N-methylpiperidine in different solvents.

Compound	pK_a (H_2O)	pK_a (DMSO)	pK_a (CH_3CN)	pK_a (THF)
pentamethylpiperidine (pmp) (protonated)			18.2[1]	
N-methylpiperidine (protonated)	10.1[2, 3]	8.4 (±1.2)[2]	18.2[2, 4]	12.9[2, 4]
N-methylindole				38.1[5] (C^2-H)
N-methylpyrrole				39.5[5] (C^2-H)
thiophene				33.0[5] (C^2-H)
phenylacetylene	23.2[6]	28.7[7]		

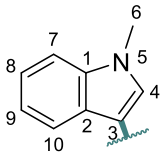
3 C(sp$^{2/3}$)-H Cleavage Experiments

General Procedure (**GP**) for the synthesis of silicates [pmpH][**2x**]:
In a *J. Young* type NMR tube (NMR scale), a crimp vial, or a Schlenk-tube, **1** (1.0 eq., synthesized according to literature known procedure[8]), substrate (1.0 eq.) and pmp (1.0 eq.) were dissolved in CD_2Cl_2 (0.45 mL, NMR scale) or CH_2Cl_2 (0.1 M), sealed, and allowed to react at the specified temperature. After the reaction proceeded, the mixture was concentrated in *vacuo* and the solid/viscous residue layered with benzene (or toluene). The mixture was shaken and allowed to settle. The solvent was separated from the residue and the step repeated two times. The residue was dried in *vacuo*.


[pmpH][2x]

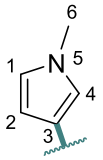
Remarks on NMR characterization: Data reported is in part taken from spectra obtained from reaction mixtures. While the NMR data is generally consistent with the isolated substances, we found occasionally minor variation in shift and multiplicity, that were neglectable for most resonances but pronounced for the NH ^{1}H-resonance (br or t, varying chemical shift).

[pmpH]**[2a]**
GP: Reaction was kept for 24 h at rt, yielding colorless crystals (182 mg, 87%; NMR scale 16 mg, 92%) suitable for scXRD (see section **7**). When conducted in toluene as solvent, direct crystallization from the reaction mixture was observed.



^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.90 (d, $^3J_{HH}$ = 8.0 Hz, 1H, ***H^7***), 7.35 (s, 1H, ***H^4***), 7.27 (d, $^3J_{HH}$ = 8.1 Hz, 1H, ***H^{10}***), 7.14 (t, $^3J_{HH}$ = 7.0 Hz, 1H, ***H^9***), 7.01 (t, $^3J_{HH}$ = 7.5 Hz, 1H, ***H^8***), 3.93 (t, $^1J_{NH}$ = 49 Hz, 1H, N***H***), 3.73 (s, 3H, indole-NC***H$_3$*** (***H^6***)), 2.61 (d, *J* = 5.8 Hz, 3H, pmp-NC***H$_3$***), 1.84 (d, *J* = 14.8 Hz, 2H, C***H$_2$***), 1.78 – 1.59 (m, 2H, C***H$_2$***), 1.51 (t, *J* = 14.0 Hz, 2H, C***H$_2$***), 1.28 (s, 6H, C(C***H$_3$***)), 1.27 (s, 6H, C(C***H$_3$***)).
^{13}C NMR [^{13}C, ^{1}H-^{13}C-HSQC, ^{1}H-^{13}C-HMBC] (151 MHz, CD_2Cl_2) δ 140.2 (***C^4***), 138.9, 134.0, 129.3, 124.2 (***C^7***), 121.0 (***C^9***), 119.5 (***C^8***), 111.3, 109.4 (***C^{10}***), 67.6 (pmp ***C***$(CH_3)_2$), 39.0 (pmp β-***C***), 33.1 (indole N***C***H_3, ***C^6***), 31.0 (pmp ***C***H_3), 30.6 (pmp N***C***H_3), 19.9 (pmp ***C***H_3), 15.8 (pmp γ-***C***).
^{19}F NMR (376 MHz, CD_2Cl_2) δ -147.4 (dd, $^3J_{FF}$ = 23.7, $^4J_{FF}$ = 6.0 Hz, 2F), -148.7 (m, 2F), -162.4 (t, $^3J_{FF}$ = 21.6 Hz, 2F), -167.1 (m, 4F), -170.3 (dt, $^3J_{FF}$ = 21.4, $^4J_{FF}$ = 7.7 Hz, 2F), -172.9 (dt, $^3J_{FF}$ = 21.4, $^4J_{FF}$ = 8.0 Hz, 2F), -176.4 (td, $^3J_{FF}$ = 21.5, $^4J_{FF}$ = 7.3 Hz, 2F), -177.7 (td, $^3J_{FF}$ = 21.5, $^4J_{FF}$ = 7.9 Hz, 2F).
^{29}Si NMR (119 MHz, CD_2Cl_2) δ -94.6.
HRMS ESI– (in CH_2Cl_2) (*m/z*) calc. for $[C_{33}H_8F_{18}N_3O_2Si]^-$ $[M]^-$, 848.0104; found 848.0104 (87%), deviation –0.1 ppm. **Elemental analysis** calc. C 51.40%, H 3.01%, N, 5.58%. found C 51.09%, H 3.13%, N 5.66%.

[pmpH]**[2b]**
GP: Reaction was kept for 48 h at rt, yielding a pale red, viscous oil. Upon grinding with a spatula, first a viscous solid was obtained, ultimately turning into a sticky, off-white powder (101 mg, 72%; NMR scale 18 mg, 80%). The reaction was also found to be successful when conducted neat (xs. N-methylpyrrole), forming a pale red to brown oil directly from the reaction mixture. Minor unassigned trace impurities were detected, possibly originating from double activation or side reactivities with the fluorinated ligand, as reported for related species [**1**−H]$^-$.[8§] Extensive extraction with benzene diminished the proportion of impurity but resulted in disproportionate yield loss.

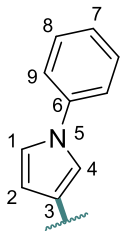


^{1}H NMR (600 MHz, CD_2Cl_2) δ 6.84 (t, *J* = 1.8 Hz, 1H, ***H^1***), 6.60 (t, $^3J_{HH}$ = 2.2 Hz, 1H, ***H^2***), 6.32 (t, $^3J_{HH}$ = 1.9 Hz, 1H, ***H^4***), 4.35 (t, $^1J_{NH}$ = 49 Hz, 1H, N***H***), 3.61 (s, ***H^6***), 2.79 (d, *J* = 5.8 Hz, 3H, pmp-NC***H$_3$***), 1.94 (d, *J* = 14.3 Hz, 2H, C***H$_2$***), 1.82 – 1.63 (m, 4H, C***H$_2$***), 1.40 (s, 6H, C(C***H$_3$***)), 1.38 (s, 6H, C(C***H$_3$***)).
^{13}C NMR [^{13}C, ^{1}H-^{13}C-HSQC, ^{1}H-^{13}C-HMBC] (151 MHz, CD_2Cl_2) δ 132.0 (***C^1***), 122.1 (***C^2***), 119.9 (***C^3***), 116.9 (***C^4***), 67.6 (pmp ***C***$(CH_3)_2$), 39.0 (pmp β-***C***), 36.1 (pyrrole-NC***H$_3$*** (***C^6***)), 30.9 (pmp ***C***H_3), 30.7 (pmp N***C***H_3), 20.0 (pmp ***C***H_3), 15.9 (pmp γ-***C***).
^{19}F NMR (376 MHz, CD_2Cl_2) δ -147.0 (dd, $^3J_{FF}$ = 23.6 Hz, $^4J_{FF}$ = 5.8 Hz, 2F), -148.9 (m, 2F), -162.7 (t, $^3J_{FF}$ = 21.5 Hz, 2F), -167.2 (t, $^3J_{FF}$ = 21.7 Hz, 2F), -167.3 (m, 2F), -170.5 (dt, $^3J_{FF}$ = 21.5 Hz, $^4J_{FF}$ = 7.8 Hz, 2F), -173.2 (dt, $^3J_{FF}$ = 21.4 Hz, $^4J_{FF}$ = 8.0 Hz, 2F), -176.7 (td, $^3J_{FF}$ = 21.5 Hz, $^4J_{FF}$ = 7.3 Hz, 2F), -178.2 (td, $^3J_{FF}$ = 21.4 Hz, $^4J_{FF}$ = 8.1 Hz, 2F).
^{29}Si NMR (119 MHz, CD_2Cl_2) δ -95.8.
HRMS ESI– (in CH_2Cl_2) (*m/z*) calc. for $[C_{29}H_6F_{18}N_3O_2Si]^-$ $[M]^-$, 797.9947; found 77.9955 (20%), deviation –1.0 ppm.

§ Of note, we observed traces of the dianion $[pmpH]_2[Si_2(am^Fph^F)_3]$ upon gas-diffusion of *n*-pentane into a solution of the title compound in CH_2Cl_2. While a clear proceeding of this reaction was not clarified yet, it might indicate an exchange of the carbanionic heteroaryl group and the ligand between silicates (e.g., 3 $[Si(am^Fph^F)_2\text{-}R]^- \rightarrow [R_3Si(am^Fph^F)]^- + [Si_2(am^Fph^F)_3]^{2-}$).

[pmpH]**[2c]**

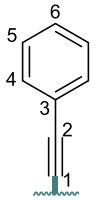
GP (NMR scale): Reaction was kept for 72 h at rt, yielding a pale red, viscous oil (22 mg, 68%). Upon grinding with a spatula, a viscous solid was obtained at first, ultimately turning into a sticky, off-white powder.



^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.44 – 7.37 (m, 4H, ***H^{Ph}***), 7.30 (br, 1H, ***H^{1}***), 7.21 (m, 1H, ***H^{Ph}***), 7.10 (t, $^{3}J_{HH}$ = 2.4 Hz, 1H, ***H^{2}***), 6.53 (br, 1H, ***H^{4}***),
4.61 (t, $^{1}J_{NH}$ = 45 Hz, 1H, N***H***), 2.81 (d, *J* = 5.5 Hz, 3H, pmp-NC***H$_3$***), 1.94 (d, *J* = 14.5 Hz, 2H, C***H$_2$***), 1.83 – 1.64 (m, 4H, C***H$_2$***), 1.43 (s, 6H, C(C***H$_3$***)), 1.38 (s, 6H, C(C***H$_3$***)).
^{13}C NMR [^{13}C, ^{1}H-^{13}C-HSQC, ^{1}H-^{13}C-HMBC] (151 MHz, CD_2Cl_2) δ 140.7 (***C^{6}***), 129.4 (***C^{Ph}*** (***C^{8}***)), 127.9 (***C^{1}***), 125.2 (***C^{7}***), 122.1 (***C^{3}***), 120.2 (***C^{Ph}*** (***C^{9}***)), 119.1 (***C^{2}***), 118.4 (***C^{4}***), 67.8 (pmp ***C***$(CH_3)_2$), 39.2 (pmp β-***C***), 31.2 (pmp ***C***H_3), 30.8 (pmp N***C***H_3), 20.0 (pmp ***C***H_3), 15.8 (pmp γ-***C***).
^{19}F NMR (376 MHz, CD_2Cl_2) δ -146.9 (dd, $^{3}J_{FF}$ = 23.7 Hz, $^{4}J_{FF}$ = 5.6 Hz, 2F), -148.9 (m, 2F), -162.6 (t, $^{3}J_{FF}$ = 21.6 Hz, 2F), -167.1 (t, $^{3}J_{FF}$ = 22.6 Hz, 2F), -167.3 (m, 2F), -170.4 (dt, $^{3}J_{FF}$ = 21.2 Hz, $^{4}J_{FF}$ = 7.8 Hz, 2F), -172.9 (dt, $^{3}J_{FF}$ = 21.5 Hz, $^{4}J_{FF}$ = 8.0 Hz, 2F), -176.5 (td, $^{3}J_{FF}$ = 21.5 Hz, $^{4}J_{FF}$ = 7.5 Hz, 2F), -178.0 (td, $^{3}J_{FF}$ = 21.5 Hz, $^{4}J_{FF}$ = 7.9 Hz, 2F).
^{29}Si NMR (119 MHz, CD_2Cl_2) δ -96.0.
HRMS ESI– (in CH_2Cl_2) (*m/z*) calc. for $[C_{34}H_8F_{18}N_3O_2Si]^-$ [M]$^-$, 860.0104; found 860.0108 (38%), deviation –0.5 ppm.

[pmpH]**[2d]**

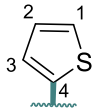
GP (NMR scale): Reaction was kept for 24 h at rt, yielding a colorless solid (37 mg, 91%).



^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.45 (m, 2H, *meta*-C_{Ph}***H*** / ***H^{5}***), 7.28 (m, 3H, *ortho*-C_{Ph}***H*** / ***H^{4}*** & *para*-C_{Ph}***H*** / ***H^{6}***), 4.58 (t, $^{1}J_{NH}$ = 49 Hz, 1H, N***H***), 2.80 (d, *J* = 5.2 Hz, 3H, pmp-NC***H$_3$***), 1.92 (d, *J* = 14.6 Hz, 2H, C***H$_2$***), 1.82 – 1.61 (m, 4H, C***H$_2$***), 1.42 (s, 6H, C(C***H$_3$***)), 1.36 (s, 6H, C(C***H$_3$***)).
^{13}C NMR [^{13}C, ^{1}H-^{13}C-HSQC, ^{1}H-^{13}C-HMBC] (151 MHz, CD_2Cl_2) δ 131.8 (***C$_{Ph}$***), 128.2 (***C$_{Ph}$***), 128.1 (***C$_{Ph}$***), 122.6 (***C$_{Ph}$***), 112.5 (***C^{sp}***), 101.6 (***C^{sp}***), 67.1 (pmp ***C***$(CH_3)_2$), 38.6 (pmp β-***C***), 30.5 (pmp ***C***H_3), 30.3 (pmp N***C***H_3), 19.6 (pmp ***C***H_3), 15.4 (pmp γ-***C***).
^{19}F NMR (565 MHz, CD_2Cl_2) δ -147.2 (dd, $^{3}J_{FF}$ = 23.3, $^{4}J_{FF}$ = 5.6 Hz, 2F), -148.8 (m, 2F), -161.5 (t, $^{3}J_{FF}$ = 21.5 Hz, 2F), -166.3 (t, $^{3}J_{FF}$ = 22.2 Hz, 2F), -166.8 (t, $^{3}J_{FF}$ = 19.5 Hz, 2F), -169.92 (d, J = 21.3 Hz, 2F), -171.78 (dt, $^{3}J_{FF}$ = 21.3 Hz, $^{4}J_{FF}$ = 7.6 Hz, 2F), -175.5 (td, $^{3}J_{FF}$ = 21.4 Hz, $^{4}J_{FF}$ = 6.6 Hz, 2F), -176.7 (td, $^{3}J_{FF}$ = 21.6 Hz, $^{4}J_{FF}$ = 7.3 Hz, 2F).
^{29}Si NMR (119 MHz, CD_2Cl_2) δ -108.4.
HRMS ESI– (in CH_2Cl_2) (*m/z*) calc. for $[C_{32}H_5F_{18}N_2O_2Si]^-$ [M]$^-$, 818.9838; found 818.9840 (38%), deviation –0.2 ppm.

[pmpH]**[2e]**

GP (NMR scale): Neat thiophene (0.4 mL) was used instead of CD_2Cl_2 as solvent, resulting in a pale red to brown oil directly from the reaction mixture. Reaction was kept for 48 h at 80 °C, yielding a pale red, viscous oil (24 mg, 78%). Upon grinding with a spatula, a viscous solid was obtained at first, ultimately turning into a sticky, off-white powder.



^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.55 (dd, $^{3}J_{HH}$ = 4.7, $^{4}J_{HH}$ = 1.0 Hz, 1H, ***H^{1}***), 7.44 (dd, $^{3}J_{HH}$ = 3.3, $^{4}J_{HH}$ = 1.1 Hz, 1H, **H^{3}**), 7.13 (dd, $^{3}J_{HH}$ = 4.7, J_{HH} = 3.4 Hz, 1H, ***H^{2}***), 4.53 (br, 1H, N***H***), 2.83 (d, *J* = 5.8 Hz, 3H, pmp-NC***H$_3$***), 1.96 (d, *J* = 14.0 Hz, 2H, C***H$_2$***), 1.86 – 1.64 (m, 4H, C***H$_2$***), 1.43 (s, 6H, C(C***H$_3$***)), 1.39 (s, 6H, C(C***H$_3$***)).
^{13}C NMR [^{13}C, ^{1}H-^{13}C-HSQC, ^{1}H-^{13}C-HMBC, DEPT-135] (101 MHz, CD_2Cl_2) δ 142.3 (***C^{4}***), 137.3 (***C^{3}***), 132.0 (***C^{1}***), 128.4 (***C^{2}***), 67.6 (pmp ***C***$(CH_3)_2$), 39.1 (pmp β-***C***), 31.0 (pmp ***C***H_3), 30.7 (pmp N***C***H_3), 20.0 (pmp ***C***H_3), 15.9 (pmp γ-***C***).
^{19}F NMR (376 MHz, CD_2Cl_2) δ -147.1 (dd, $^{3}J_{FF}$ = 23.2, $^{4}J_{FF}$ = 5.9 Hz, 2F), -148.9 (m, 2F), -162.0 (t, $^{3}J_{FF}$ = 21.5 Hz, 2F), -166.8 (t, $^{3}J_{FF}$ = 22.3 Hz, 2F), -167.1 (m, 2F), -170.1 (dt, $^{3}J_{FF}$ = 21.5 Hz, $^{4}J_{FF}$ = 7.6 Hz, 2F), -172.31 (dt, $^{3}J_{FF}$ = 21.4 Hz, $^{4}J_{FF}$ = 7.9 Hz, 2F), -175.9 (td, $^{3}J_{FF}$ = 21.4 Hz, $^{4}J_{FF}$ = 7.0 Hz, 2F), -177.2 (td, $^{3}J_{FF}$ = 21.4 Hz, $^{4}J_{FF}$ = 7.5 Hz, 2F).
^{29}Si NMR (79 MHz, CD_2Cl_2) δ -99.8.
HRMS ESI– (in CH_2Cl_2) (*m/z*) calc. for $[C_{28}H_3F_{18}N_2O_2SSi]^-$ [M]$^-$, 800.9403; found 800.9396 (100%), deviation 0.8 ppm.

4 Determination of the Kinetic Isotope Effect

For the determination of the kinetic isotope effect N-methylindole was considered as a suitable substrate due to a fast and clean reaction and its regioselectivity (only reactivity in 3-position observed). 3-deutero-N-methylindole was prepared according to a literature known procedure (> 97% deuteration in 3-position).[9]
In a *J Young* type NMR tube, equimolar amounts of 3-deutero-N-methylindole and N-methylindole (1.0 eq., 80 µmol, each) were dissolved in CD_2Cl_2 together with pmp (1.0 eq.) and hexamethylbenzene as internal standard (1.0 eq.). The mixture was analyzed by NMR spectroscopy. ^{1}H NMR experiments were conducted with a relaxation time of 60 s, to preclude misleading quantifications caused by incomplete integration data. Subsequently, **1** (1.0 eq.) was added and the reaction allowed to proceed for 12 h at rt. ^{19}F and ^{29}Si NMR spectroscopy confirmed full conversion of the FLP **1**/pmp. Assuming that the consumed substrate was fully converted to the respective silicate, a KIE (k_H/k_D) can be calculated from this data as shown below (**Scheme S1**, uncertainty calculated assuming an integral error of 0.01 with *Gaussian* error propagation).

Calculation of the KIE
When using an intermolecular experiment, commonly equimolar amounts of deuterated and protonated substrate are reacted and the KIE is calculated as a ratio of the yield derived from the protonated to the deuterated form.[10] The present experiment was planned accordingly, yet the exact ratio of protonated to deuterated form was determined using NMR integrals and the calculation therefore modified accordingly, using the yields referenced against the initial substrate (formula **(I)**, **Scheme S1**).

$$\textbf{(I)}\quad KIE = \frac{k_H}{k_D} = \frac{\frac{[P_H]_{t>0}}{[S_H]_{t=0}}}{\frac{[P_D]_{t>0}}{[S_D]_{t=0}}} = \frac{[P_H]_{t>0}}{[S_H]_{t=0}} \bullet \frac{[S_D]_{t=0}}{[P_D]_{t>0}}$$

$$\textbf{(II)}\quad KIE = \frac{[S_H]_{t=0} - [S_H]_{t>0}}{[S_H]_{t=0}} \bullet \frac{[S_{H+D}]_{t=0} - [S_H]_{t=0}}{\left([S_{H+D}]_{t=0} - [S_{H+D}]_{t>0}\right) - \left([S_H]_{t=0} - [S_H]_{t>0}\right)}$$

$$\textbf{(i)}\quad [S_D]_{t=0} = [S_{H+D}]_{t=0} - [S_H]_{t=0}$$

$$\textbf{(ii)}\quad [P_H]_{t>0} = [S_H]_{t=0} - [S_H]_{t>0}$$

$$\textbf{(iii)}\quad [P_D]_{t>0} = [P_{H+D}]_{t>0} - [P_H]_{t>0} = \left([S_{H+D}]_{t=0} - [S_{H+D}]_{t>0}\right) - \left([S_H]_{t=0} - [S_H]_{t>0}\right)$$

Scheme S1. Formulas for the calculation of the KIE. $[S_{H/D}]_t$ – concentration of protonated (H) or deuterated substrate (D) at given time x; $[S_{H+D}]_t$ – total, combined concentration of protonated **and** deuterated substrate at given time t; time t = 0 – prior to reaction, before the addition of Lewis acid; time t > 0 – after reaction proceeded.

Calibrating the spectra to the solvent signal and the integral for the internal standard at a constant value, the signals at 6.5 ppm, 7.2 ppm and 7.6 ppm were integrated, as all were judged sufficiently separated from neighboring resonances prior to and after the reaction proceeded. The resonance at 6.5 ppm represents the hydrogen involved in the cleavage process, the resonances at 7.2 ppm and 7.6 ppm both serve as estimation for the combined concentration of N-methylindole substrate (deuterated and protonated) and were averaged for the final KIE assessment. Relative values of the integrals are listed in **Table S2**, corresponding spectra are shown in **Figure S1**.

Table S2. Resonances and integrals used for the assessment of the KIE. Signals were integrated in a range of ±0.1 ppm when no neighboring signal was found in this range or otherwise to the maximal possible range.

	Integrated Signal [ppm]	Integral Value	Proportional To
t = 0	6.5 (***H*^{3}** of substrate)	1.088	$[S_H]_{t=0}$
t = 12 h		0.378	$[S_H]_{t>0}$
t = 0	7.6 (***H*^{4}** of substrate)	2.147	$[S_{H+D}]_{t=0}$
t = 12 h		1.240	$[S_{H+D}]_{t>0}$

The final KIE was calculated utilizing formula **(II)** (**Scheme S1**). Instead of the molar concentrations, integral values of respective ^{1}H NMR signals were utilized directly (**Table S2**), which are proportional to the molar concentrations. The latter might be derived through multiplication with the concentration of the internal standard.

Ultimately, a KIE of 3.5 can be assessed. It shall be noted that the present experiment is intended to give qualitative proof for a direct involvement of the C-H/D bond in the rate-determining step and does not serve as exact quantification of kinetic data. An assumed integral uncertainty of 0.01 propagates to an uncertainty of ±0.7 of the final KIE (not considering used approximations and possible systematic errors).

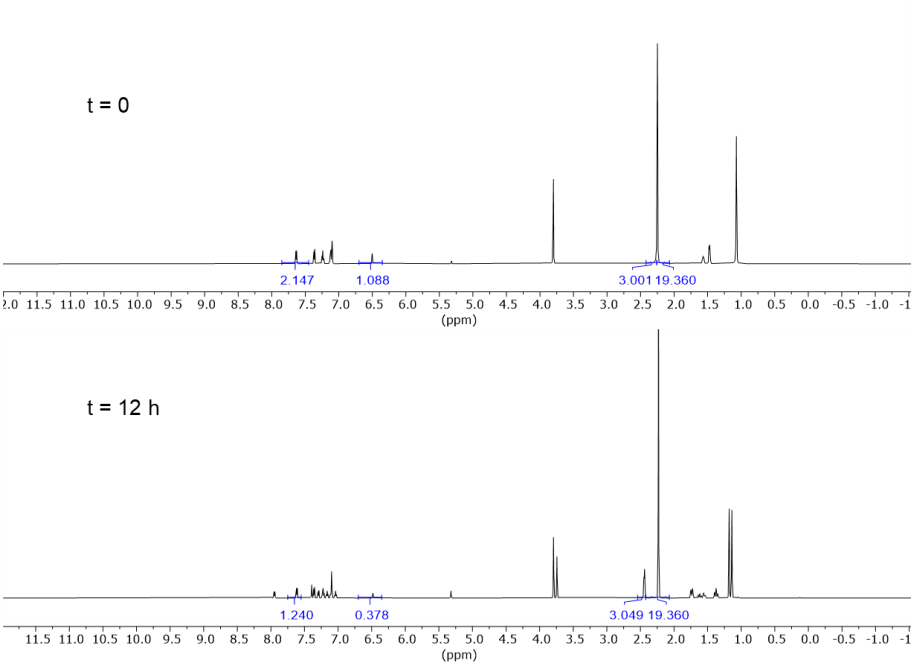


Figure S1. ^{1}H NMR spectra with the respective integrals for the determination of the kinetic isotope effect in the CH bond cleavage of N-methylindole by **1** and pmp.

5 Donor Induced Reversal of the Bond Cleavage

To a solution of [pmpH][**2a**] (11 mg) in CD_2Cl_2 (0.45 mL) was added an equimolar amount of 1,3-Dimethyl-2-imidazolidinone (DMI) and the mixture was monitored using NMR spectroscopy. After 48 h at rt signals of N-methylindole in ^{1}H NMR spectra indicated a donor induced reversal of the bond cleavage (31%[§]). Heating of the mixture to 60 °C accelerated the process and led to 91%[§] conversion of the initial silicate after 40 h (**Figure S2**).
Apart from N-methylindole, **1**-DMI was identified as main product through comparison of ^{19}F NMR spectra (**Figure S3** and paragraph below). Minor unassigned signals (< 5%, assuming a structural relation to the am^{F}ph^{F} ligand system) are partially also found upon addition of DMI to unbound **1** and might correspond to a possible bis-adduct.

1-DMI
To a solution of unbound **1** (13 mg) in CD_2Cl_2 was added 1 eq. DMI. NMR spectroscopy indicated adduct formation. The connectivity of the adduct was further confirmed by scXRD analysis of poor-quality crystals that formed upon gas diffusion of *n*-pentane into the reaction mixture (see **Figure S5**, full refinement prevented by problems related to superstructures). Yield was not determined.

^{1}H NMR (600 MHz, CD_2Cl_2) δ 3.55 (br, 4H, C***H*****$_2$**), 2.81 (s, 6H, C***H*****$_3$**).
^{13}C NMR (151 MHz, CD_2Cl_2) δ 45.9 (***C****H*$_3$), 31.4 (br, ***C****H*$_2$).
CO signal was not detected.
^{19}F NMR (565 MHz, CD_2Cl_2) δ -147.3 (br, 2F), -148.4 (br, 2F), -158.9 (t, $^{3}J_{FF}$ = 21.5 Hz, 2F), -164.9 (br, 2F), -165.3 (br, 2F), -167.8 (dd, $^{3}J_{FF}$, $^{4}J_{FF}$ = 21.1, 9.1 Hz, 2F), -170.0 (dd, $^{3}J_{FF}$, $^{4}J_{FF}$ = 21.1, 9.1 Hz, 2F), -172.3 (td, $^{3}J_{FF}$, $^{4}J_{FF}$ = 21.3, 5.4 Hz, 2F), -173.2 (td, $^{3}J_{FF}$, $^{4}J_{FF}$ = 21.2, 5.8 Hz, 2F).
^{29}Si NMR (119 MHz, CD_2Cl_2) δ -109.8.

[§] Conversions determined through internal integration in ^{1}H NMR spectra.

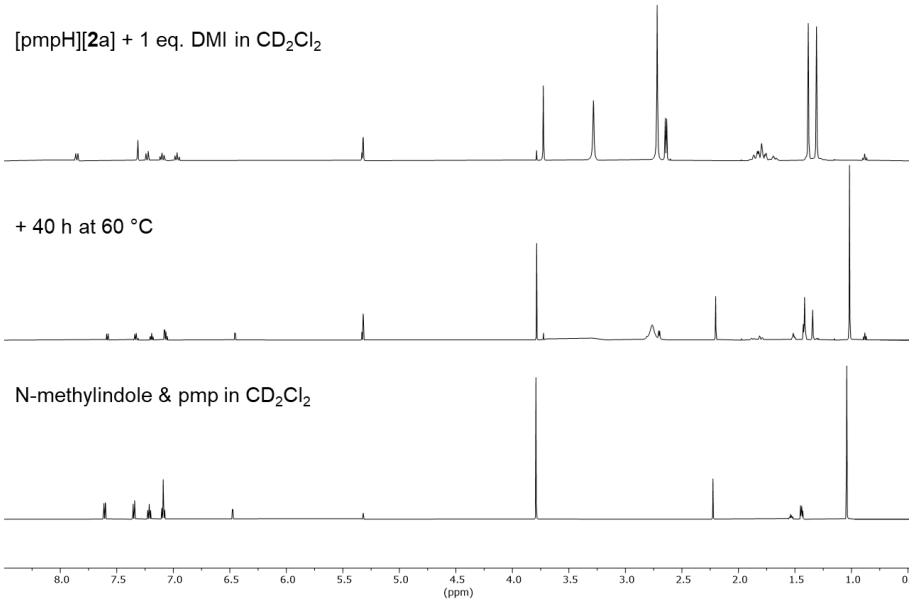


Figure S2. Stacked ^{1}H NMR spectra for the monitoring of the donor-induced reverse reaction of the CH bond cleavage.

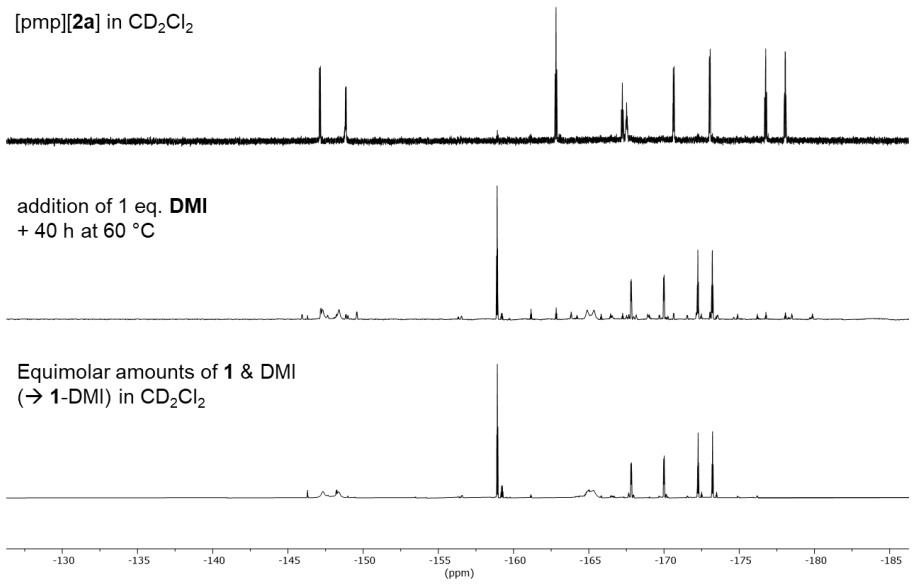
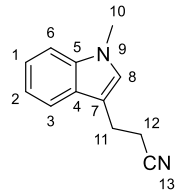


Figure S3. Stacked ^{19}F NMR spectra for the monitoring of the donor-induced reverse reaction of the CH bond cleavage.

6 Reactivity and Catalysis

Catalysis – General procedure.
A *J. Young* type NMR tube was charged with 10 mol% catalyst (10 µmol), heteroarene (1.0 – 5.0 eq.) and CD_2Cl_2 (0.45 mL). Cyclooctane (100 µmol, 1 eq.) was added as internal standard for the determination of yields by internal integration. Acrylonitrile (1.0 – 3.0 eq.) was added, the tube capped, kept at rt under constant motion and the mixture was continuously monitored using ^{1}H NMR spectroscopy. When the reaction had proceeded, aq. sat. Na_2CO_3 solution was added, the phases separated, and the aqueous phase extracted with DCM (x2). The combined organic phases were dried over Na_2SO_4 and filtered over a short pad of silica, eluting with DCM. The solvent was removed under reduced pressure and the residue rigorously dried in *vacuo*.

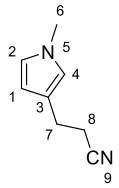
3a (3-(N-methylpyrrole-3-yl)-propionitrile).
1.0 eq. N-methylindole, 3.0 eq. acrylonitrile. After 3 d at rt internal integration revealed >99% of product formation. Pale yellow viscous (87%).



^{1}H NMR (200 MHz, CD_2Cl_2) δ 7.56 (d, J_{HH} = 7.7 Hz, 1H), 7.34 (d, J = 8.1 Hz, 1H), 7.24 (t, J_{HH} = 7.4 Hz, 1H), 7.12 (t, J_{HH} = 7.3 Hz, 1H), 7.02 (s, 1H), 3.76 (s, 3H), 3.12 (t, J_{HH} = 7.1 Hz, 2H), 2.72 (t, J_{HH} = 7.1 Hz, 2H).
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 (dd, J_{HH} = 7.9, 0.9 Hz, 1H, ***H^3***), 7.34 (dd, J_{HH} = 8.2, 0.9 Hz, 1H, ***H^6***), 7.28 (tt, J_{HH} = 9.0, 1.6 Hz, 1H, ***H^1***), 7.16 (tt, J_{HH} = 6.9, 1.2 Hz, 1H, ***H^2***), 7.01 (s, 1H, ***H^8***), 3.78 (s, 3H, ***H^{10}***), 3.13 (t, J_{HH} = 7.2 Hz, 2H, ***H^{11}***), 2.70 (t, J_{HH} = 7.2 Hz, 2H, ***H^{12}***).

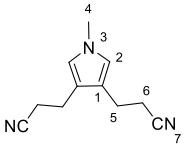
NMR data is consistent with the one found in literature.[11]
^{13}C NMR [^{13}C, ^{1}H-^{13}C-HSQC, ^{1}H-^{13}C-HMBC] (151 MHz, $CDCl_3$) δ 137.1 (***C^5***), 127.1 (***C^4***), 127.0 (***C^8***), 122.0 (***C^1***), 119.9 (***C^{13}***), 119.3 (***C^2***), 118.3 (***C^3***), 111.1 (***C^7***), 109.6 (***C^6***), 32.8 (N***C***H_3, ***C^{10}***), 21.7 (***C^{11}***), 19.0 (***C^{12}***).
GCMS EI+ *Retention time* 14.5 min. *m/z* 184.18 (26%) [M]+, 144.14 (100%) [M – $CNCH_2$]$^+$.

3b (3-(N-methylpyrrole-3-yl)-propionitrile).
5.0 eq. N-methylpyrrole, 1.0 eq. acrylonitrile. After 14 h at rt internal integration revealed 86% of product formation. Pale yellow viscous (75%). Minor formation of **3b'** was observed (5% according to internal integration).



^{1}H NMR (200 MHz, $CDCl_3$) δ 6.59 (t, J_{HH} = 2.3 Hz, 1H), 6.08 (t, J_{HH} = 3.2 Hz, 1H), 5.99 (m, 1H), 3.58 (s, 3H), 2.95 (t, J_{HH} = 7.5 Hz, 3H), 2.65 (t, J_{HH} = 7.3 Hz, 3H).
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.59 (d, J_{HH} = 4.4 Hz, 1H, ***H^2***), 6.08 (d, J_{HH} = 6.3 Hz, 1H, ***H^1***), 5.98 (ddd, J_{HH} = 2.6, 1.7, 0.9 Hz, 1H, ***H^4***), 3.58 (s, 3H), 2.95 (td, J_{HH} = 7.6, 3.0 Hz, 4H, ***H^7***), 2.65 (t, J_{HH} = 7.6 Hz, 2H, ***H^8***).
^{13}C NMR [^{13}C, ^{1}H-^{13}C-HSQC, ^{1}H-^{13}C-HMBC] (101 MHz, $CDCl_3$) δ 129.0 (***C^3***), 122.5 (***C^2***), 119.3 (***C^9***), 107.2 (***C^1***), 106.6 (***C^4***), 33.7 (***C^6***), 22.7 (***C^7***), 17.4 (***C^8***).
GCMS EI+ *Retention time* 11.5 min. *m/z* 134.30 (24%) [M]+, 94.25 (100%) [M – $CNCH_2$]$^+$.

3b' (3,3'-(N-methylpyrrole-3,4-diyl)-dipropionitrile).
1.0 eq. N-methylpyrrole, 3.0 eq. acrylonitrile. After 3 d at rt internal integration revealed 92% of product formation. Pale orange solid (80%).



^{1}H NMR (200 MHz, CD_2Cl_2) δ 5.92 (s, 2H, ***H^2***), 3.43 (s, 3H, ***H^4***), 2.92 (t, J_{HH} = 7.2 Hz, 4H, ***H^5***), 2.65 (t, J_{HH} = 7.0 Hz, 4H, ***H^6***).
^{1}H NMR [^{13}C, ^{1}H-^{13}C-HSQC, ^{1}H-^{13}C-HMBC] (600 MHz, $CDCl_3$) δ 5.93 (s, 2H, ***H^2***), 3.46 (s, 3H, ***H^4***), 2.93 (t, J_{HH} = 7.5 Hz, 4H, ***H^5***), 2.64 (t, J_{HH} = 7.5 Hz, 4H, ***H^6***).
^{13}C NMR (151 MHz, $CDCl_3$) δ 129.5 (***C^1***), 119.2 (***C^7***), 105.7 (***C^2***), 30.4 (***C^4***), 23.0 (***C^5***), 17.2 (***C^6***).
GCMS EI+ *Retention time* 16.4 min. *m/z* 187.18 (28%) [M]+, 147.18 (90%) [M – $CNCH_2$]$^+$, 107.17 (100%) [M – $CNCH_2$ − CN]$^+$.

Reaction of [pmpH][2a] with acrylonitrile.
Reacting a solution of equimolar amounts [pmpH]**[2a]** in CD_2Cl_2 at rt revealed formation of 38% **3a** after 16 h (determined by internal ^{1}H integration and GCMS measurements). Longer reactions times up to 14 d only revealed a minorly increased proportion of **3a**.

Comparison experiments with different silanes.
A *J. Young* type NMR tube was charged with N-methylpyrrole (21 µmoL), equimolar amounts of silane (**1**, $Si(cat^{Cl})_2$,[12] $SiCl_4$) as well as pmp, and the compounds mixed in CD_2Cl_2. The reaction mixtures were monitored using NMR spectroscopy. Conversions mentioned in the main manuscript were obtained through integration of ^{1}H NMR spectra after addition of hexamethylbenzene as internal standard.

7 Computational Details

All geometry optimizations and single point energies were calculated using the Orca 5.0 program package.[13, 14] As starting geometries, VSEPR structures preoptimized with UFF were used. Geometry optimizations for all compounds were performed with the PBE0 functional,[15, 16] utilizing *Grimme's* semi-empirical dispersion correction[17] (D3), the *Becke-Johnson* damping function[18-20] (BJ), and the def2-TZVPP basis set,[21, 22] using *defgrid2* settings. All calculated equilibrium structures have been confirmed as energetic minima on the potential energy surface by analytical calculation of harmonic frequencies at the level of optimization, revealing only positive Hessian eigenvalues. Transition geometries were optimized toward a single negative Hessian matrix eigenvalue. It was ensured that the correct first-order saddle point on the potential energy surface was located by animation of the imaginary frequency in Chemcraft.[23] Enthalpies at 298.15 K have been calculated by using the rigid-rotor harmonic oscillator (RRHO) approximation,[24] as implemented in Orca. In all computations, the resolution-of-identity[25] and "chain of spheres"[26] approximation in the form of RIJCOSX was used in combination with matching auxiliary basis sets.[27] Final single point energies for the structures were obtained at the DLPNO-CCSD(T)/def2-TZVPP level of theory.[21, 22, 28-31] Implicit solvation effects were considered at this level using the *Universal Solvent Model* (SMD),[32] as implemented in the Orca program package.[33] This combination is denoted as DLPNO-CCSD(T)/def2-TZVPP+SMD(CH_2Cl_2)//PBE0-D3(BJ)/def2-TZVPP in the main text. Resulting energies as well as thermodynamic and kinetic data are summarized in **Table S3**.

Table S3. Computed energies for the calculation of thermodynamics and kinetics. Note that concentration contribution from gas phase (1 atm.) to solution phase (1 mol L^{-1}) for the solvation was considered (ΔE^0_{conc} = RT•ln(24.5) = 7.9 kJ mol^{-1}, for T = 298K).

	PBE0-D3(BJ)/def2-TZVPP			DLPNO-CCSD(T)/ def2-TZVPP SMD(CH_2Cl_2)	G = ($E^{DLPNO} - E^{PBE0} + G^{PBE0}$) + ΔE^0_{conc}
Compound	**E^{PBE0} [a.u.]**	**G^{PBE0} [a.u.]**	**H^{PBE0} [a.u.]**	**E^{DLPNO} [a.u.]**	**G [kJ mol^{-1}]**
1	-3259.3246	-3259.1694	-3259.0636	-3256.7757	-8550250.0
pmp	-448.0953	-447.8317	-447.7829	-447.6534	-1174614.1
$[pmpH]^+$	-448.5023	-448.2241	-448.1747	-448.1345	-1175839.2
[**1**····pmp]^{VDW}	-3707.4480	-3707.0044	-3706.8727	-3704.4546	-9724873.6
N-methylindole	-402.8151	-402.6894	-402.6480	-402.4032	-1056171.5
[2a]$^-$ / [**1**-$C_9H_5NCH_3^{C3\text{-}pos.}$]$^-$	-3661.6797	-3661.3855	-3661.2624	-3658.7465	-9605259.5
1····$C_9H_6NCH_3^{C3\text{-}pos.}$ (**INT-2a**)	-3662.1568	-3661.8479	-3661.7263	-3659.1977	-9606405.5
[TS-a-$FLP^{C2\text{-}pos.}$]‡	-4110.2442	-4109.6491	-4109.5033	-4106.8349	-10780925.6
[TS-a-$FLP^{C3\text{-}pos.}$]‡	-4110.2632	-4109.6663	-4109.5219	-4106.8595	-10780985.6
Thermodynamics					**ΔG**
[**1**····pmp]^{VDW} + N-methylindole --> **[2a]$^-$** + $[pmpH]^+$					-53.6
[**1**····pmp]^{VDW} + N-methylindole --> **1**····$C_9H_6NCH_3^{C3\text{-}pos.}$ + pmp					25.5
Kinetics					**ΔG**
[**1**····pmp]^{VDW} + N-methylindole --> [TS-a-$FLP^{C2\text{-}pos.}$]‡					119.5
[**1**····pmp]^{VDW} + N-methylindole --> [TS-a-$FLP^{C3\text{-}pos.}$]‡					59.5
N-methylpyrrole	-249.2839	-249.2019	-249.1666	-249.0409	-653633.8
[2b]$^-$ / [**1**—$C_4H_3NCH_3^{C3\text{-}pos.}$]$^-$	-3508.1445	-3507.8959	-3507.7772	-3505.3821	-9202721.0
1····$C_4H_4NCH_3^{C3\text{-}pos.}$ (**INT-2b**)	-3508.6232	-3508.3608	-3508.2425	-3505.8287	-9203856.9
[TS-b-$FLP^{C2\text{-}pos.}$]‡	-3956.7192	-3956.1688	-3956.0278	-3953.4817	-10378413.8
[TS-b-$FLP^{C3\text{-}pos.}$]‡	-3956.7252	-3956.1755	-3956.0343	-3953.4891	-10378435.3
[TS-b-ELC-$O^{C2\text{-}pos.}$]‡	-3508.5774	-3508.3192	-3508.2022	-3505.7758	-9203729.1
[TS-b-ELC-$O^{C3\text{-}pos.}$]‡	-3508.5765	-3508.3190	-3508.2016	-3505.7769	-9203733.8
[TS-b-ELC-$N^{C2\text{-}pos.}$]‡	-3508.5760	-3508.3188	-3508.2008	-3505.7739	-9203727.0
[TS-b-ELC-$N^{C3\text{-}pos.}$]‡	-3508.5749	-3508.3183	-3508.2000	-3505.7750	-9203731.4
Thermodynamics					**ΔG**
[**1**····pmp]^{VDW} + N-methylpyrrole --> **[2b]$^-$** + $[pmpH]^+$					−52.8
[**1**····pmp]^{VDW} + N- methylpyrrole --> **1**····$C_4H_4NCH_3^{C3\text{-}pos.}$ + pmp					36.4
Kinetics (FLP)					**ΔG**
[**1**····pmp]^{VDW} + N- methylpyrrole --> [TS-b-$FLP^{C2\text{-}pos.}$]‡					93.6
[**1**····pmp]^{VDW} + N- methylpyrrole --> [TS-b-$FLP^{C3\text{-}pos.}$]‡					72.1
Kinetics (ELC)					**ΔG**
[**1**····pmp]^{VDW} + N- methylpyrrole --> [TS-b-ELC-$O^{C2\text{-}pos.}$]‡ + pmp					164.2
[**1**····pmp]^{VDW} + N- methylpyrrole --> [TS-b-ELC-$O^{C3\text{-}pos.}$]‡ + pmp					159.6
[**1**····pmp]^{VDW} + N- methylpyrrole --> [TS-b-ELC-$N^{C2\text{-}pos.}$]‡ + pmp					166.3
[**1**····pmp]^{VDW} + N- methylpyrrole --> [TS-b-ELC-$N^{C3\text{-}pos.}$]‡ + pmp					162.0
thiophene	-552.7634	-552.7235	-552.6913	-552.2663	-1449862.5
[2e]$^-$ / [**1**—$C_4H_3S^{C2\text{-}pos.}$]$^-$	-3811.6307	-3811.4236	-3811.3084	-3808.6127	-9998961.6
[**1**—$C_4H_3S^{C3\text{-}pos.}$]$^-$	-3811.6267	-3811.4202	-3811.3044	-3808.6076	-9998950.3
[TS-e-$FLP^{C2\text{-}pos.}$]‡	-4260.1957	-4259.6898	-4259.5504	-4256.7027	-11174637.7
[TS-e-$FLP^{C3\text{-}pos.}$]‡	-4260.1879	-4259.6807	-4259.5425	-4256.6951	-11174614.2

Thermodynamics					**ΔG**
[**1**⋯pmp]^{VDW} + thiophene --> **[2e]**$^{-}$ + [pmpH]$^{+}$					−64.7
[**1**⋯pmp]^{VDW} + thiophene --> [**1**—$C_4H_3S^{C3\text{-}pos.}$]$^{-}$ + [pmpH]$^{+}$					−53.4
Kinetics (FLP)					**ΔG**
[**1**⋯pmp]^{VDW} + thiophene --> [TS-e-FLP$^{C2\text{-}pos.}$] ‡					98.4
[**1**⋯pmp]^{VDW} + thiophene --> [TS-e-FLP$^{C3\text{-}pos.}$] ‡					121.9
phenylacetylene (PhCCH)	-308.1402	-308.0605	-308.0228	-307.8239	-807974.5
[2d]$^{-}$ / [**1**-CCPh]$^{-}$	-3567.0122	-3566.7658	-3566.6437	-3564.1757	-9357089.0
1—PhCCH	-3567.4713	-3567.2112	-3567.0912	-3564.5982	-9358162.4
Thermodynamics					**ΔG**
[**1**⋯pmp]^{VDW} + PhCCH --> **[2d]**$^{-}$ + [pmpH]$^{+}$					−80.1
[**1**⋯pmp]^{VDW} + PhCCH --> [**1**—PhCCH·]$^{-}$ + [pmpH]$^{+}$					71.7
$SiCl_4$	-2129.8583	-2129.8835	-2129.8435	-2128.1797	-5587594.6
pmp-$SiCl_4$	-2577.9019	-2577.6350	-2577.5706	-2575.7864	-6762019.1
[TS-N-methylpyrrole--pmp-$SiCl_4$] ‡	-2827.2050	-2826.8399	-2826.7603	-2824.8439	-7415661.8
Thermodynamics					
$SiCl_4$ + pmp --> pmp-$SiCl_4$					189.6
Kinetics					
$SiCl_4$ +pmp + N-methylpyrrole --> [TS-N-methylpyrrole--pmp-$SiCl_4$] ‡					180.7
$Si(cat^{Cl})_2$	-4727.7242	-4727.6717	-4727.5971	-4723.9832	-12402672.9
pmp-$Si(cat^{Cl})_2$	-5175.8413	-5175.4947	-5175.3970	-5171.6652	-13577290.3
[TS-N-methylpyrrole--pmp-$Si(cat^{Cl})_2$]‡	-5425.1240	-5424.6786	-5424.5665	-5420.6961	-14230861.4
[$Si(cat^{Cl})_2$⋯pmp]^{VDW} (van-der-Waals adduct)	-5175.8359	-5175.4953	-5175.3940	-5171.6494	-13577264.5
$Si(cat^{Cl})_2$⋯$C_4H_4NCH_3$	-4977.0220	-4976.8625	-4976.7750	-4973.0387	-13056287.3
[$Si(cat^{Cl})_2$—$C_4H_4NCH_3{}^{C3\text{-}pos.}$]$^{-}$	-4976.5412	-4976.3951	-4976.3069	-4972.5914	-13055148.4
[$Si(cat^{Cl})_2$—$C_4H_4NCH_3{}^{C2\text{-}pos.}$]$^{-}$	-4976.5429	-4976.3966	-4976.3086	-4972.5895	-13055142.6
Thermodynamics[§]					**ΔG**
$Si(cat^{Cl})_2$ + pmp --> pmp-$Si(cat^{Cl})_2$					-3.3
$Si(cat^{Cl})_2$ + pmp --> [$Si(cat^{Cl})_2$⋯pmp]^{VDW}					22.5
$Si(cat^{Cl})_2$ + N-methylpyrrole --> $Si(cat^{Cl})_2$⋯$C_4H_4NCH_3$					19.5
$Si(cat^{Cl})_2$ + N-methylpyrrole + pmp --> [pmpH]$^{+}$ + [$Si(cat^{Cl})_2$—$C_4H_4NCH_3{}^{C2\text{-}pos.}$]$^{-}$					-61.0
$Si(cat^{Cl})_2$ + N-methylpyrrole + pmp --> [pmpH]$^{+}$ + [$Si(cat^{Cl})_2$—$C_4H_4NCH_3{}^{C3\text{-}pos.}$]$^{-}$					-66.8
Kinetics[§]					**ΔG**
$Si(cat^{Cl})_2$ + N-methylpyrrole + pmp --> [TS-N-methylpyrrole--pmp-$Si(cat^{Cl})_2$]‡					62.7

[§] Energies derived are calculated using the monomeric $Si(cat^{Cl})_2$ structure due to computational ease. It shall be noted that the donor-free form is not monomeric and undergoes oligomerization.[12] It is reported that the oligomerization is easily reversed in presence of donors and the in *silico* consideration of a monomer leads to reasonable results,[34] yet deviations to the calculations using a monomeric form are to be expected.

8 Single Crystal X-Ray Diffraction (scXRD)

General

For scXRD measurements, a suitable crystal was picked from the mother liquor, immersed in perfluorinated polyether oil, and fixed on top of a cryo loop. A Bruker APEX-III CCD diffractometer with a low-temperature unit using Mo-Kα radiation, chromated by mirror optics, was used for phi- and omega- scans. Data acquisition was done at 100.0 K. A strategy for data collection was calculated with Bruker's APEX3 software. The same program was used for processing of collected data. Data reduction, scaling, and absorption corrections were done with SAINT. SA-DABS-2016/2 was used for multi-scan absorption correction. Structures were solved with dual methods as implemented in the ShelXT 2018 structure solution program. Structure refinement was carried out by full matrix least squares minimization on F2 using the 2018/3 version of ShelXL. All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using a riding model. Handling of the structural data during solution and refinement was performed with the Olex2 v1.3 graphical interface.[35]

For data visualization, Mercury 4.1.3 was used.[36-38] The thermal displacement ellipsoids are shown at the probability level of 50%.

CCDC 2279861 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre's and FIZ Karlsruhe's joint Access Service *via* https://www.ccdc.cam.ac.uk/structures/?.

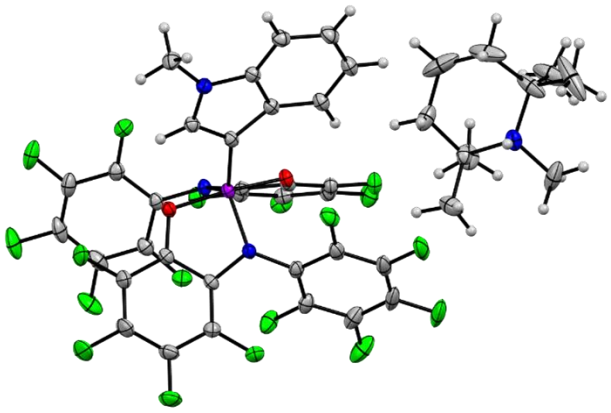


Figure S4. Solid state molecular structure of [pmpH][**2a**]. Ellipsoids are drawn with a probability of 50%.

Table S4. Crystal data for [pmpH][**2a**].

CCDC number	2279861
Empirical formula	$C_{43}H_{30}F_{18}N_4O_2Si$
Formula weight	1004.80
Temperature [K]	100.00
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	19.1013(6)
b [Å]	11.5155(3)
c [Å]	19.3079(6)
α [°]	90
β [°]	105.8930(10)
γ [°]	90
Volume [Å^3]	4084.6(2)
Z	4
ρ_{calc} [gcm^{-3}]	1.634
μ [mm^{-1}]	0.185
F(000)	2032
Crystal size [mm^3]	0.412×0.383×0.295
Crystal color	colorless
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.17 to 56.71 (0.75 Å)
Index ranges	−25 ≤ h ≤ 25 −15 ≤ k ≤ 15 −25 ≤ l ≤ 25
Reflections collected	106718
Independent reflections	10124 R_{int} = 0.0412 R_{sigma} = 0.0198
Completeness to θ = 25.242°	99.1 %
Data / Restraints / Parameters	10124/0/619
Goodness-of-fit on F^2	1.027
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0425 wR_2 = 0.1074
Final *R* indexes [all data]	R_1 = 0.0456 wR_2 = 0.1099
Largest peak/hole [eÅ^{-3}]	0.86/-0.62

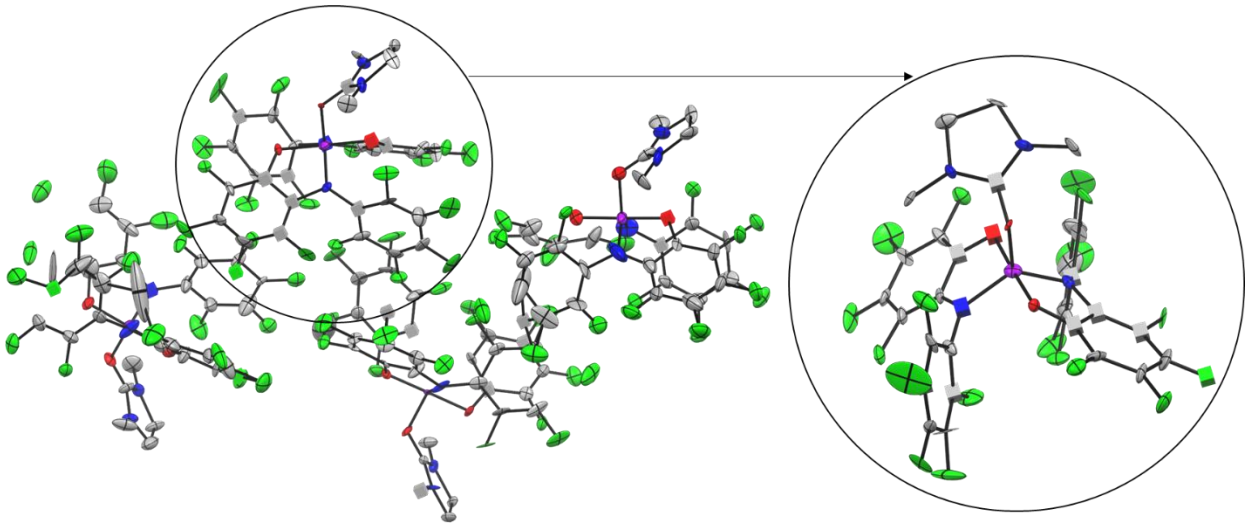


Figure S5. Unrefined solid state molecular structure of **1**-DMI. Ellipsoids are drawn with a probability of 50%.

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10 Spectra

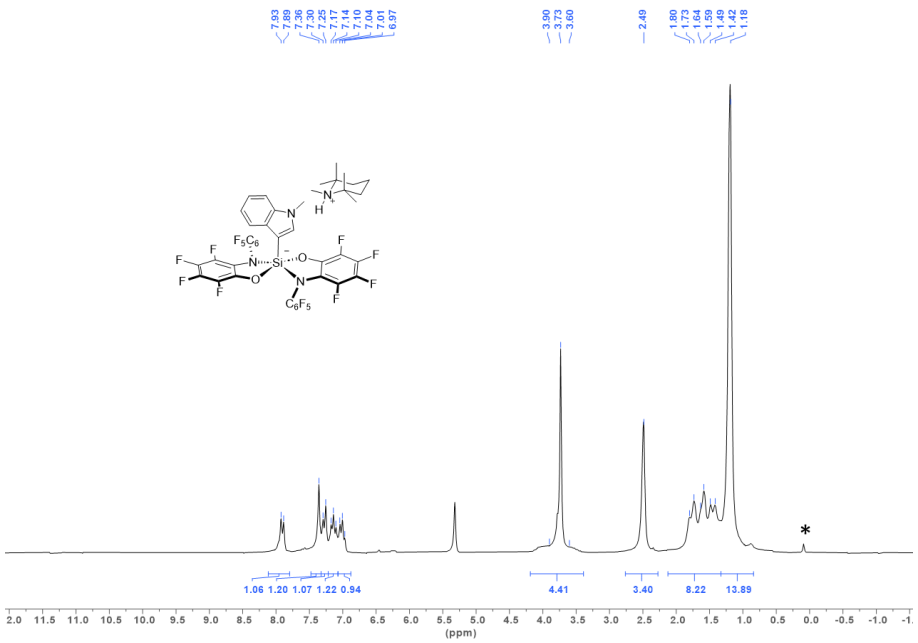

Figure S6. ^{1}H NMR (200 MHz, CD_2Cl_2) spectrum of [pmpH][**2a**]. Residual silicon-grease resonance is marked with an asterisk.

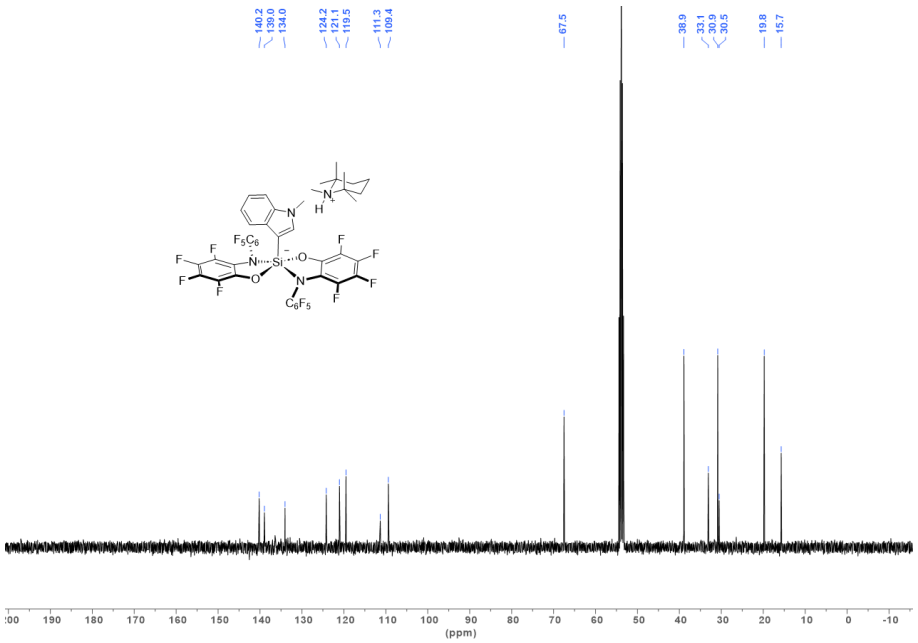

Figure S7. ^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of [pmpH][**2a**].

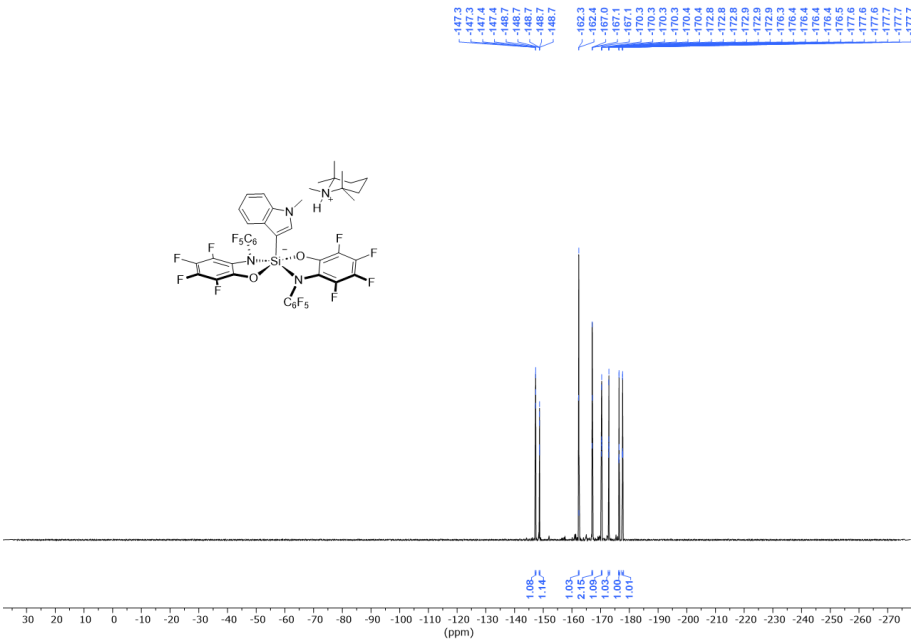

Figure S8. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of [pmpH][**2a**].

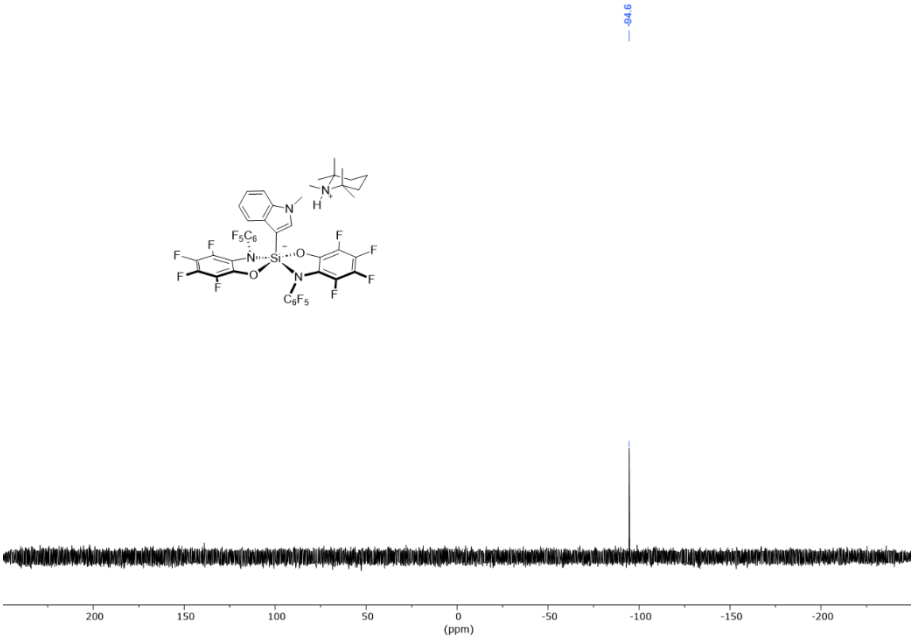

Figure S9. ^{29}Si NMR (119 MHz, CD_2Cl_2) spectrum of [pmpH][**2a**].

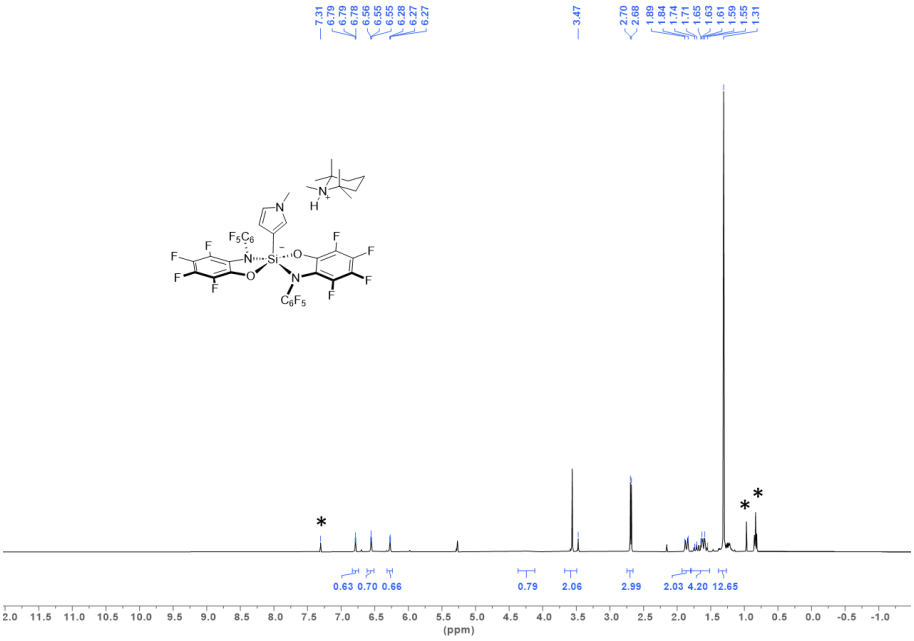

Figure S10. ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of [pmpH][**2b**]. Residual H-grease and C_6H_6 resonances are marked with an asterisk.

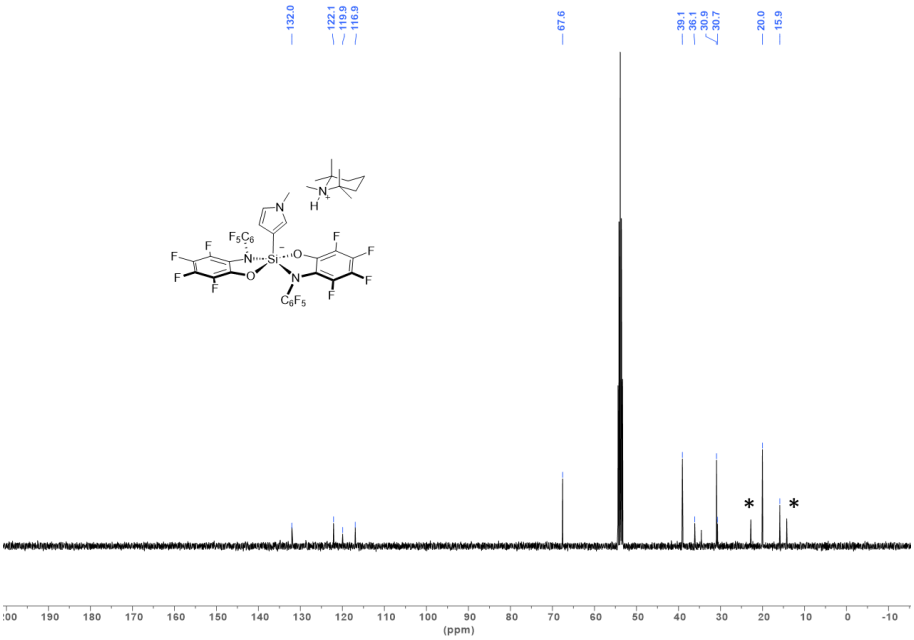

Figure S11. ^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of [pmpH][**2b**]. Residual H-grease resonances are marked with an asterisk.

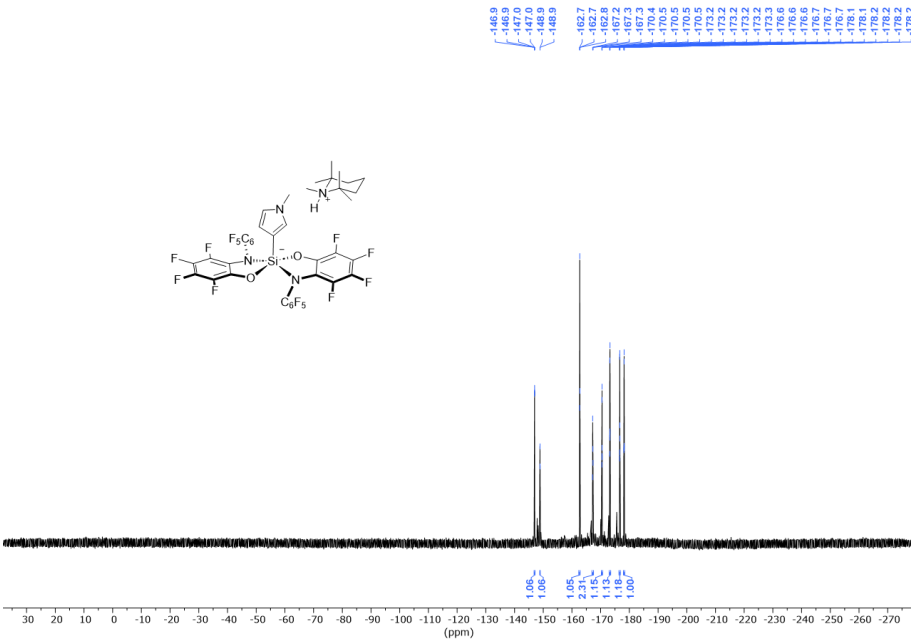

Figure S12. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of [pmpH][**2b**].

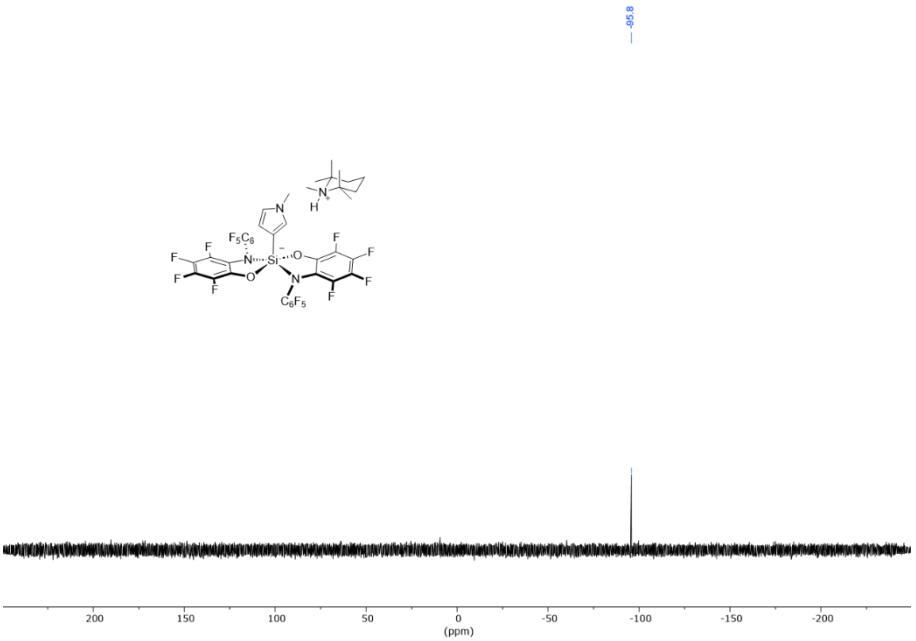

Figure S13. ^{29}Si NMR (119 MHz, CD_2Cl_2) spectrum of [pmpH][**2b**].

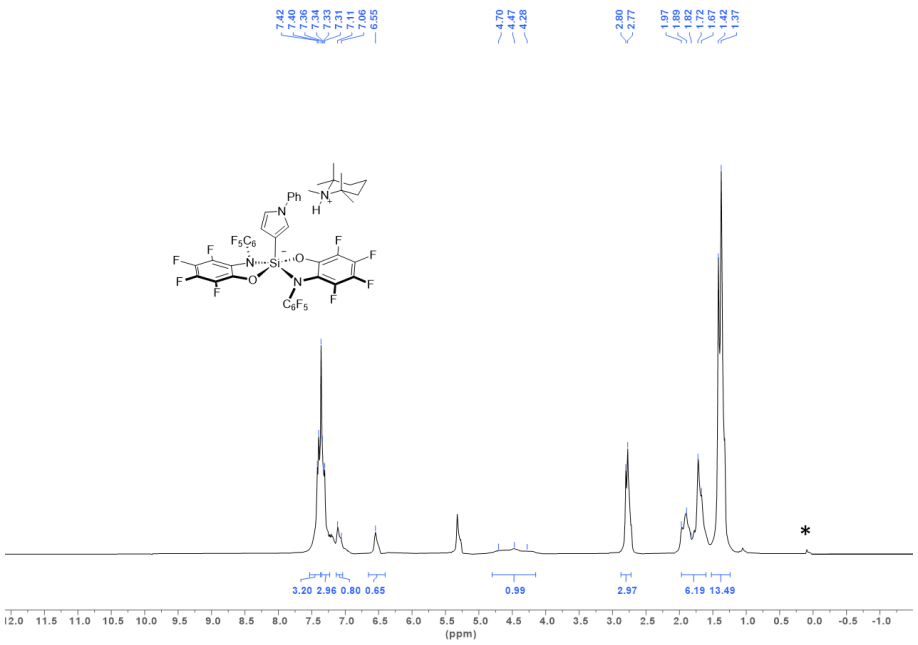

Figure S14. ^{1}H NMR (200 MHz, CD_2Cl_2) spectrum of [pmpH][**2c**]. Residual silicon-grease resonance is marked with an asterisk.

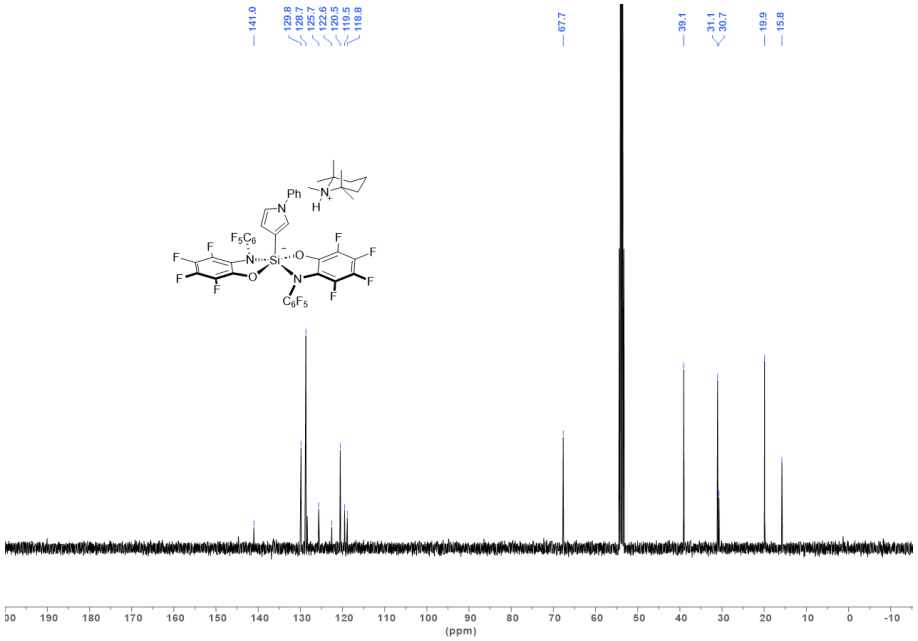

Figure S15. ^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of [pmpH][**2c**].

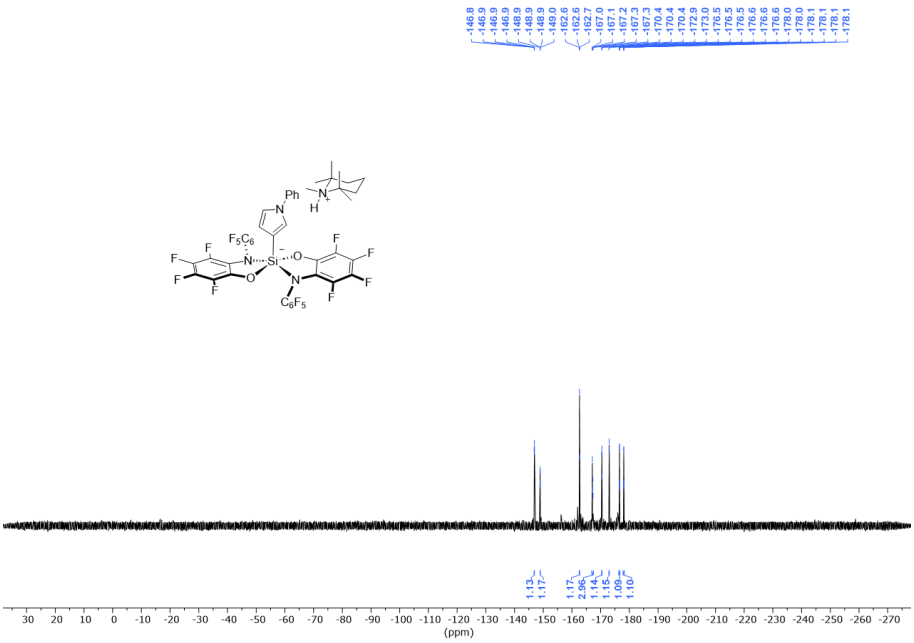

Figure S16. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of [pmpH][**2c**].

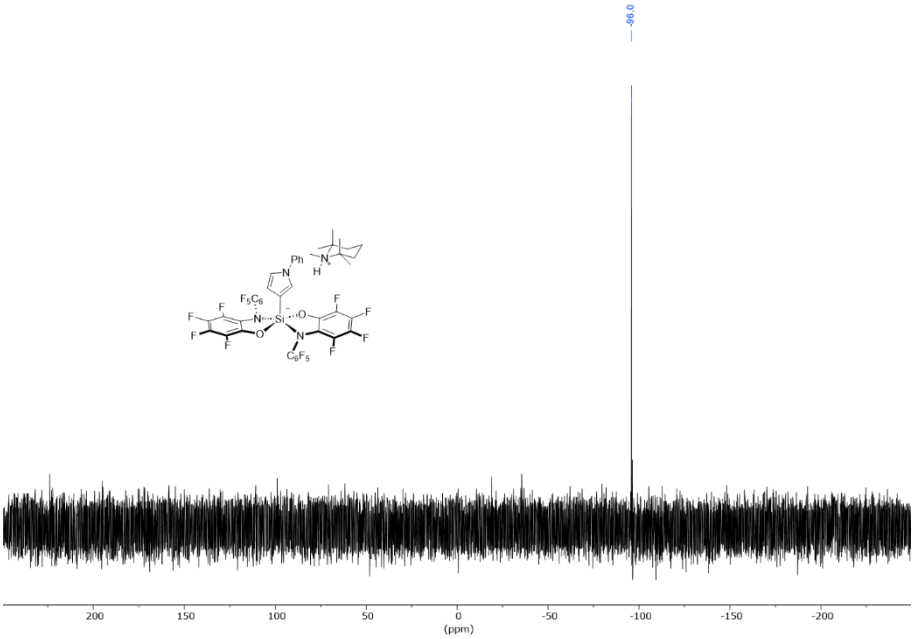

Figure S17. ^{29}Si NMR (119 MHz, CD_2Cl_2) spectrum of [pmpH][**2c**].

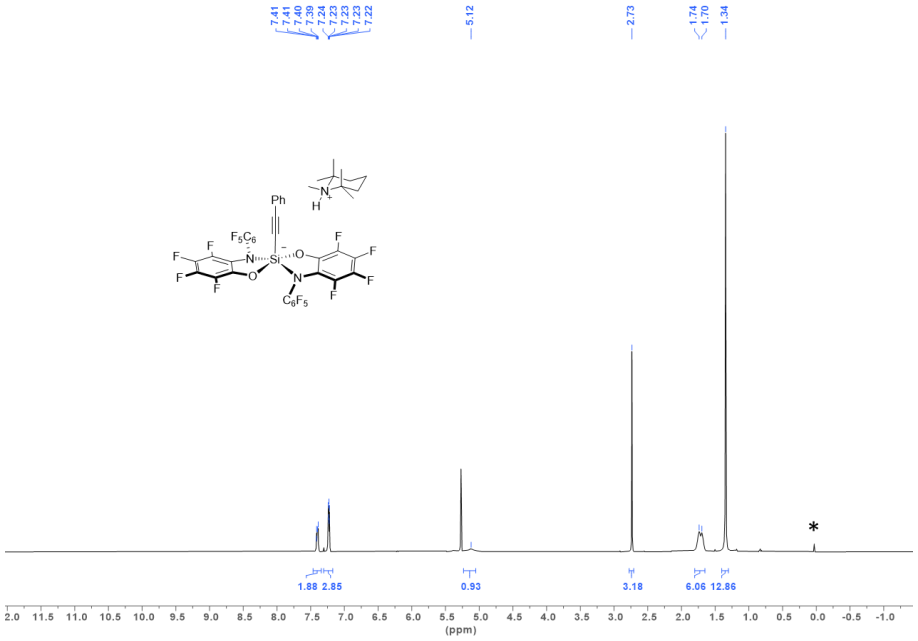

Figure S18. ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of [pmpH][**2d**]. Residual silicon-grease resonance is marked with an asterisk.

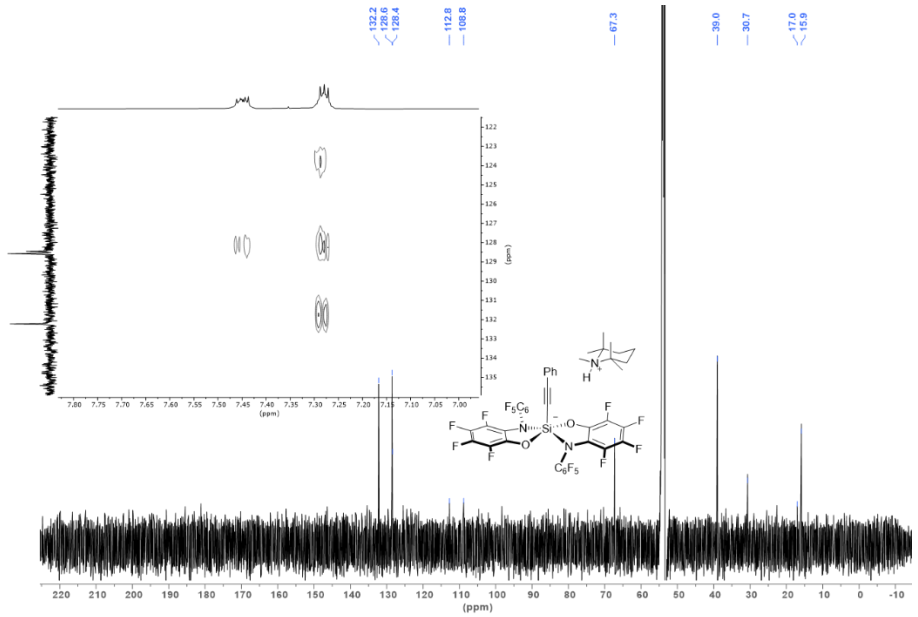

Figure S19. ^{13}C NMR (101 MHz, CD_2Cl_2) and ^{1}H-^{13}C-HMBC spectra of [pmpH][**2d**].

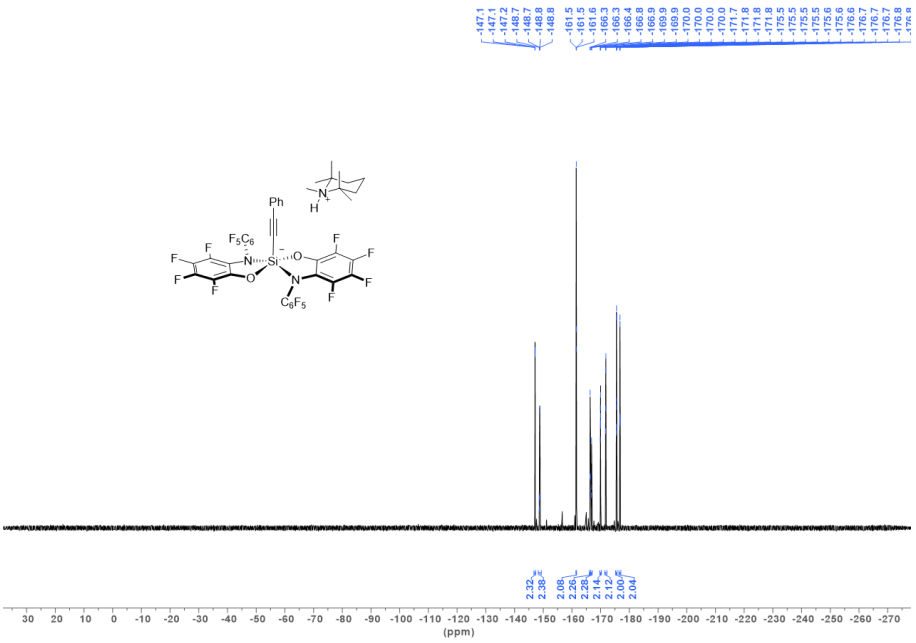

Figure S20. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of [pmpH][**2d**].

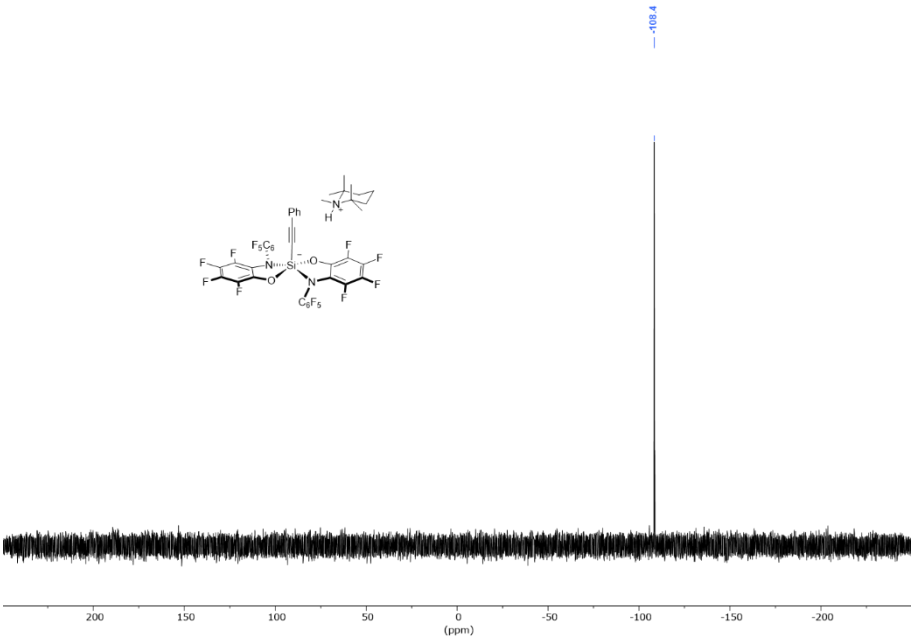

Figure S21. ^{29}Si NMR (119 MHz, CD_2Cl_2) spectrum of [pmpH][**2d**].

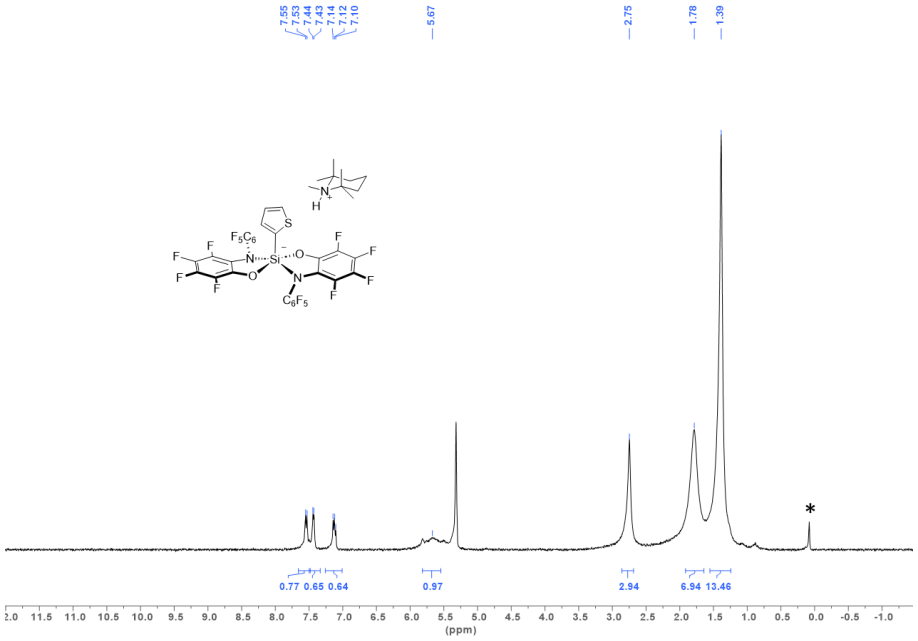

Figure S22. ^{1}H NMR (200 MHz, CD_2Cl_2) spectrum of [pmpH][**2e**]. Residual silicon-grease resonance is marked with an asterisk.

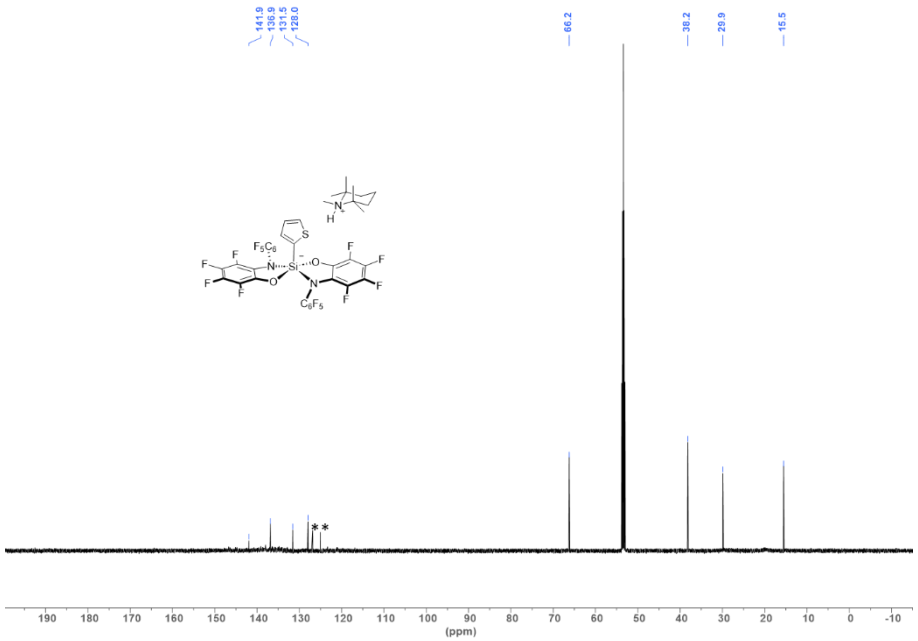

Figure S23. ^{13}C NMR (151 MHz, CD_2Cl_2) spectrum of [pmpH][**2e**]. Residual thiophene resonances are marked with an asterisk.

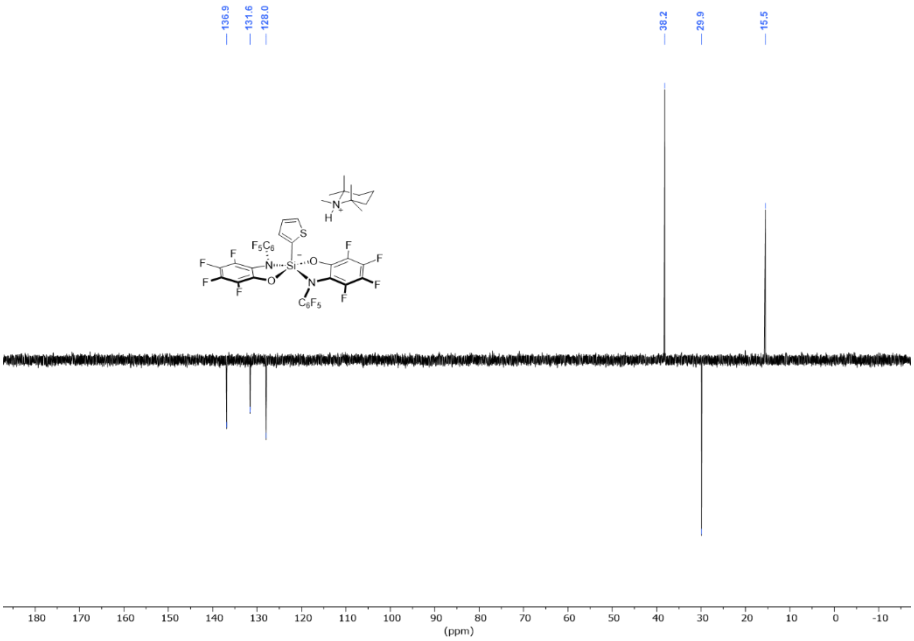

Figure S24. ^{13}C NMR (101 MHz, CD_2Cl_2) spectrum of [pmpH][**2e**].

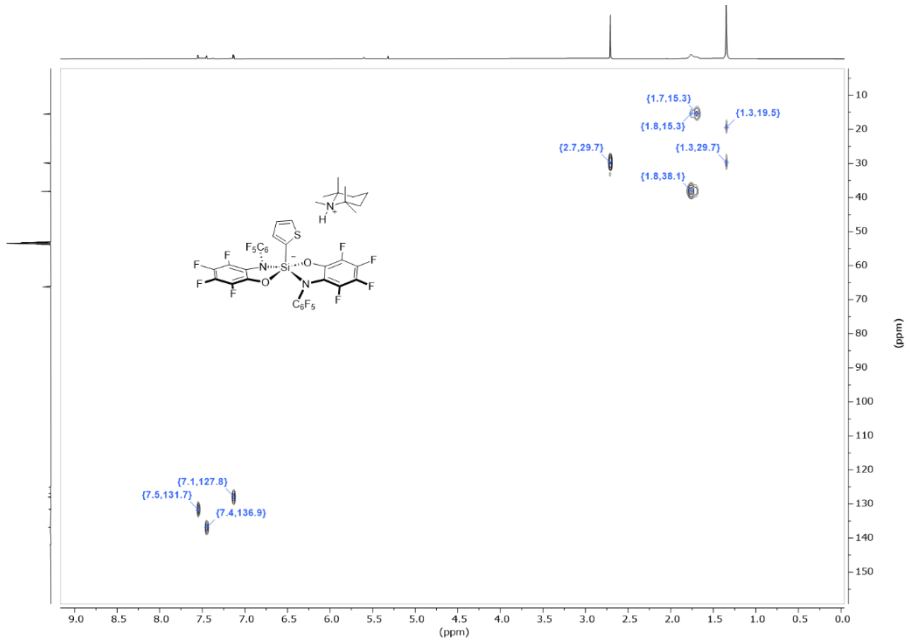

Figure S25. ^{1}H-^{13}C-HSQC (600/151 MHz, CD_2Cl_2) spectrum of [pmpH][**2e**].

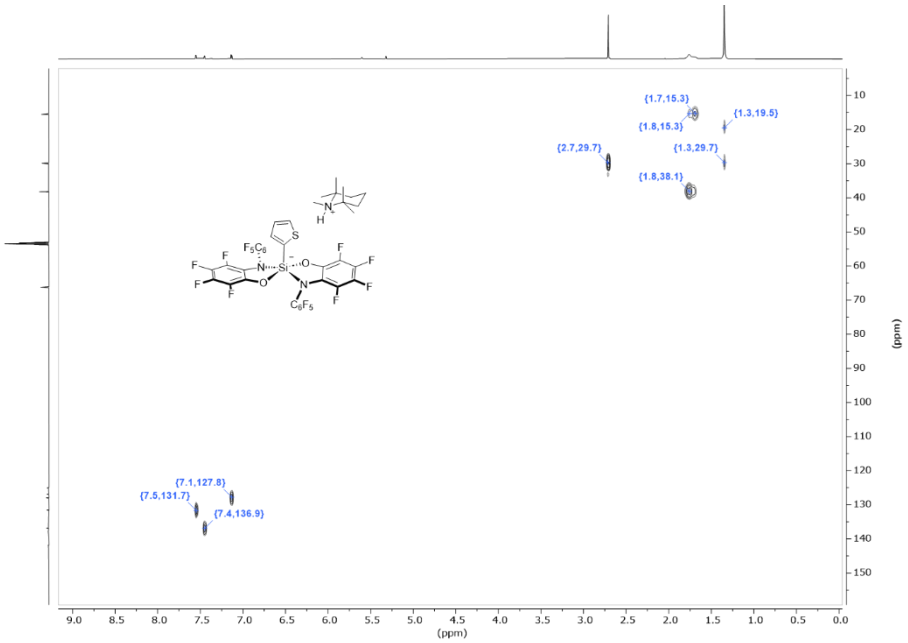

Figure S26. ^{1}H-^{13}C-HMBC (600/151 MHz, CD_2Cl_2) spectrum of [pmpH][**2e**].

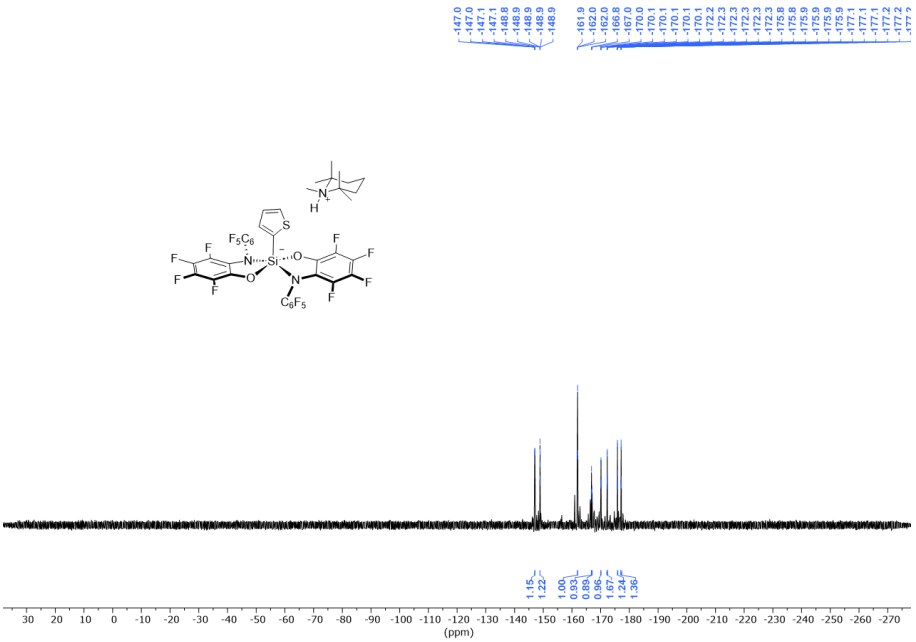

Figure S27. ^{19}F NMR (376 MHz, CD_2Cl_2) spectrum of [pmpH][**2e**].

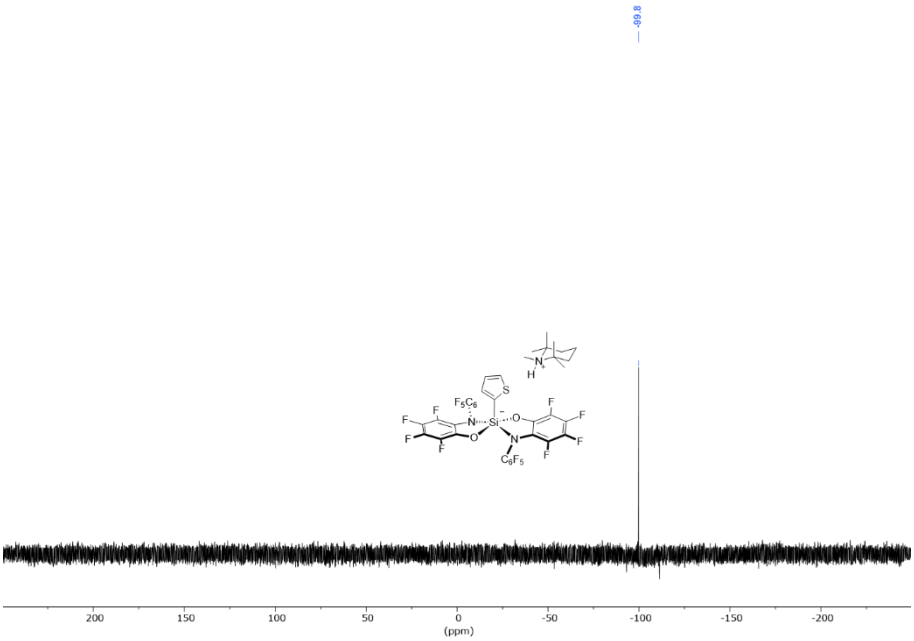

Figure S28. ^{29}Si NMR (119 MHz, CD_2Cl_2) spectrum of [pmpH][**2e**].

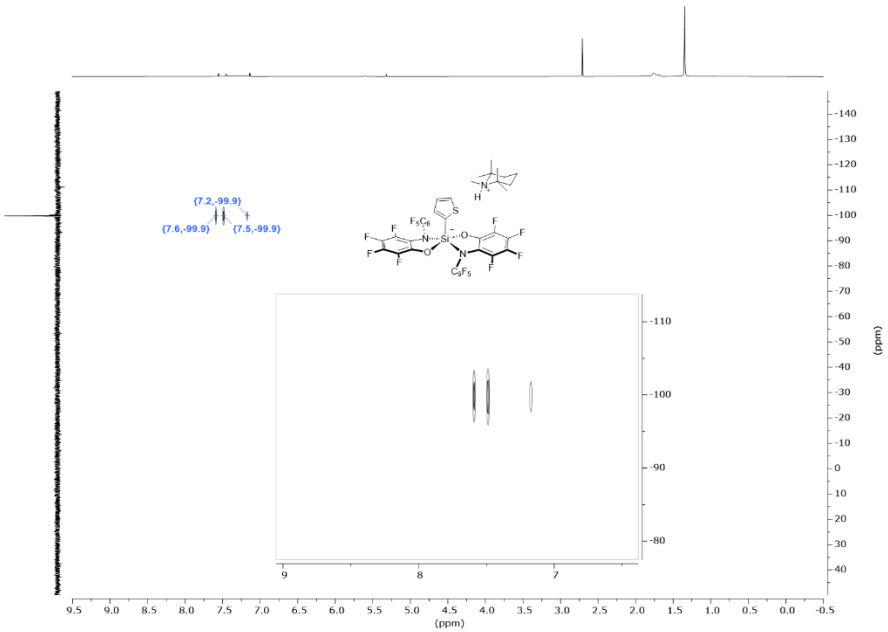

Figure S29. ^{1}H-^{29}Si-HMBC (600/119 MHz, CD_2Cl_2) spectrum of [pmpH][**2e**].

11 Cartesian Coordinates of Computed Structures (XYZ Format)

For coordinates of **1**, pmp, $[pmpH]^+$, and $[\mathbf{1}\cdots pmp]^{vdW}$ see previous work with calculations on the same level of theory.[8]

N-methylindole

C	-5.18395143130943	0.39541490645733	-0.24280155909141
C	-3.92849446019029	0.83895516035491	0.05331439892577
C	-4.06518637912635	2.18507615364646	0.50940524771795
H	-3.01748610532484	0.27118467447318	-0.04258724560119
N	-6.10571562718461	1.38313021625341	-0.00153583312398
H	-5.50911450937269	-0.56409341495320	-0.61384061602925
C	-5.44633798485158	2.49128420298209	0.46106240276067
C	-3.17417178902152	3.16461734802059	0.95459303994708
C	-5.94667834133584	3.73258365503840	0.84130305019152
C	-7.52360508526574	1.28531958908027	-0.19638075045932
H	-8.06075061519562	1.43388847149961	0.74382808615048
H	-7.76351554972008	0.29476139229552	-0.57800179807003
H	-7.87273723625009	2.02843820986883	-0.91753393332219
C	-5.03888367269656	4.67857851255161	1.27691266840179
C	-3.66694067502163	4.39719866931246	1.33290356458779
H	-2.11136633560992	2.95874764800137	1.00232993946763
H	-2.98479754761022	5.16369764445364	1.67969721770491
H	-7.00625691650512	3.95380260012780	0.80008212454939
H	-5.39373973840783	5.65576436053569	1.58052999529239

[2a]$^-$

C	-5.09076857506450	2.45362674731919	-0.39131196506676
C	-5.85799999462540	1.40225364379949	-0.84887563329834
C	-3.89301895104893	2.21067461469908	0.27340949496759
F	-5.49268487039566	3.71284132508952	-0.59095624659236
C	-5.43617806203106	0.09360490980577	-0.63775951728246
F	-7.00099695944164	1.64190151645770	-1.49699533282777
C	-4.25400345476496	-0.15306175536053	0.03078556514861
C	-3.46891917800366	0.91444623248580	0.49811191385794
N	-2.30387200142987	0.44113351666836	1.07551516878273
F	-3.16854008766559	3.26903132332895	0.66414089918020
F	-6.18266178848667	-0.91720735638268	-1.09350460448752
O	-3.75033508133984	-1.35390641204192	0.25638939237630
C	-1.47492699450461	1.29599743211897	1.80693491475897
C	-1.88569563261398	1.83075809225486	3.02409259728619
C	-1.06267970886955	2.64419274710350	3.78162204014492
F	-3.10272563976052	1.56348854030566	3.48199758437881
C	0.21414540180336	2.93316380324925	3.33359803699900
F	-1.48723062713057	3.14227279963384	4.93962680066182
C	0.65016851237505	2.41586588604726	2.12567425191526
F	1.01447347551294	3.70891241507420	4.05828189150278
C	-0.19423722314693	1.61985554714484	1.37234055440368
F	1.87348621545809	2.69732695529694	1.68985081334691
F	0.24659002202260	1.16808509453476	0.20790429804115
Si	-2.16429904821597	-1.36646943762298	1.07065347618899
O	-0.49336160552248	-1.22444592028485	1.64119460819008
N	-1.47614071790668	-2.32439092892121	-0.30923107795171
C	0.41280776042317	-1.81906827140393	0.88489481585895
C	-0.10144004878650	-2.48036783502994	-0.24242739840791
C	-2.24352471018716	-3.10963193023368	-1.17318312284736
C	1.77115572511803	-1.79969931928943	1.12594639743297
F	2.26150078698580	-1.16533521470283	2.19499114759464
C	2.64276016963278	-2.43467954325227	0.24804346153851
C	0.77541294193822	-3.09436648779284	-1.11672988274729
C	2.14501158026767	-3.07399584075508	-0.86888210387921
F	0.34808401963553	-3.71046455787504	-2.22873854535458
F	3.95746238687540	-2.42287528788534	0.48402904216009
F	2.98102539321672	-3.66861861158410	-1.72548352296454
C	-2.92544940455251	-2.55328293911508	-2.25062732155882
C	-2.40197286652005	-4.47596665093225	-0.95969848735514
C	-3.74617466154368	-3.31350329086088	-3.06529273195831
F	-2.79918499002518	-1.26282483270440	-2.52010053949954
C	-3.88705136296679	-4.66991313927553	-2.82648180352366
C	-3.20772246558377	-5.25410272204672	-1.77180681264802
F	-4.39210150605371	-2.75186821460228	-4.08217615413022
F	-4.66781071097534	-5.41036229668992	-3.60800921464830
F	-1.77238303115593	-5.06238508803881	0.05086225377163
F	-3.34336931966543	-6.55702177483829	-1.53814782731280
C	-2.78312509251299	-2.31552731436064	2.54103130106103
C	-4.07412175691558	-2.77186879982916	2.64861711027056
N	-4.26258407463643	-3.48653198324189	3.79934595346298
C	-3.07842789716437	-3.51602438670067	4.49099483362133
C	-2.12168555512975	-2.79276254876524	3.73694091247724
C	-5.48432234787884	-4.10045115541034	4.22526006566836
H	-6.25813830419523	-3.89861391465105	3.48685894440602
H	-5.81087012095222	-3.69982193866681	5.18913364791721
H	-5.36955831606076	-5.18381928067844	4.32253661799709
C	-2.78850716660279	-4.11876182145562	5.70966637235878
C	-1.49827564148671	-3.99327115013274	6.19007242315263
C	-0.82923000065227	-2.68160264572889	4.25971090872159
C	-0.53318157155134	-3.28015115427839	5.47022153949538
H	-3.54183380067943	-4.66703690910325	6.26324202035442
H	-0.07523150074285	-2.12566040083662	3.72133106014379
H	0.46981015074295	-3.19509724504186	5.87161439885667
H	-1.23237283113930	-4.45110932762346	7.13563670588415
H	-4.89167728372220	-2.63758550638999	1.95799361000456

1$\cdots C_9H_6NCH_3^{C3\text{-}pos.}$

C	-5.79735232002904	1.40863323916330	-0.16777711207822
C	-6.34984313454740	0.16591190096495	-0.42167314933636
C	-4.49559256369983	1.52035604621268	0.31027885051374
F	-6.51201714751388	2.50511838697550	-0.38957318900037
C	-5.59737611688241	-0.97994453664835	-0.20047101120559
F	-7.59149175717130	0.06678096093461	-0.88086098238334
C	-4.30740753303217	-0.87107388781014	0.27704765175388
C	-3.74302279339337	0.38332558758784	0.54939620309768
N	-2.42822241082707	0.24749710682893	0.98918122573669
F	-4.00091918484767	2.74171571618848	0.51034523699751
F	-6.12176808351833	-2.17861530940433	-0.46236360606203
O	-3.49397401299304	-1.91064476898521	0.46875236170606
C	-1.74102791221572	1.31069961400562	1.59095957565858
C	-2.24364320094844	1.95240979822844	2.71719376735602
C	-1.57091886479216	2.99013004187330	3.33356502367178
F	-3.41090502541360	1.55600351576059	3.22815946147442
C	-0.33793993684030	3.38828750123106	2.84359607013929
F	-2.09105930881176	3.59295544137277	4.39213805703043
C	0.20008591857969	2.75147833013772	1.73653536296504
F	0.32100259632182	4.37123348930980	3.43361061190099
C	-0.50341608917815	1.73203631644612	1.11717921731831
F	1.37847463752269	3.12970843362492	1.26840313041782
F	0.02997322889940	1.14698863529005	0.05631654154494
Si	-1.95306298997991	-1.45701502196713	1.12400934643811
O	-0.41374495553265	-1.14924088197642	1.84601427915606
N	-1.11929833373264	-2.47620060992925	-0.06436310412183
C	0.61796982370567	-1.73463003994346	1.22584789357314
C	0.26034299604636	-2.51305429030783	0.12048684081055
C	-1.74179968629637	-3.17008149606975	-1.11355612936423
C	1.93707716326633	-1.58806217297307	1.60048999907277
F	2.26894013615428	-0.82843224526579	2.64020595497157
C	2.92818763733100	-2.23030781773182	0.86785697087714
C	1.25470662915074	-3.13888590080146	-0.60982797571641
C	2.58467870244829	-3.00202494215246	-0.22725319780071
F	0.98375146581756	-3.86842874893042	-1.69345931976130
F	4.20379143828795	-2.09736900290409	1.21255043951325
F	3.53318616691728	-3.61642055419316	-0.92508931850470
C	-2.41505468660230	-2.48322418712012	-2.11701641364634
C	-1.76121957160254	-4.55798829624614	-1.16834159354061
C	-3.11757599852744	-3.14381486225760	-3.10803637956876
F	-2.41534516308776	-1.15652238577826	-2.11950826716230
C	-3.12749791883099	-4.52890891968316	-3.13384957061421
C	-2.43771938394373	-5.23791429788985	-2.16502008756417
F	-3.77948168469794	-2.45934410770138	-4.02836206135823
F	-3.78990590192883	-5.17231869629730	-4.08102067268603
F	-1.11580501136745	-5.26160334303574	-0.24900838219074
F	-2.43721623774918	-6.56327676919326	-2.18880087190582
C	-2.54050788434297	-2.05655092042088	3.09250865801313
C	-3.92452841648184	-1.78524949201309	3.18970773073049
N	-4.63014374840103	-2.88546641991434	2.98365510852184
C	-3.77570433420437	-3.97641905937700	2.82697029096050
C	-2.45952575447495	-3.51264207361780	2.96219838718600
C	-6.06404332314866	-2.95511590441350	2.82910999255223
H	-6.49213475525947	-1.97928799604446	3.04440485193336
H	-6.47418908469510	-3.69193293691689	3.51933085395676
H	-6.31054887701545	-3.23624950508469	1.80525387350330
C	-4.08548185140486	-5.30672415711027	2.59305423485979
C	-3.02312347157841	-6.19031183399973	2.53348178361625
C	-1.40689240260049	-4.41865050678211	2.89876039794965
C	-1.70554369875655	-5.75298879165916	2.69640205525453
H	-5.10526074861783	-5.64455870458131	2.46303099622890
H	-0.38105674802454	-4.08584034727906	2.99352472824764
H	-0.90099351226544	-6.47482908361965	2.64134853517212
H	-3.21519870268194	-7.24001627144848	2.35362157353150

H	-1.82258778316151	-1.46456366522714	3.64368159668757
H	-4.40909852279812	-0.83169429942999	3.33775407297091

[TS-a-FLP$^{C2\text{-}pos.}$]‡

C	-5.75211683330626	2.96240464516117	-0.46943786533443
C	-6.54853557064883	1.83806684540096	-0.59290604061770
C	-4.52643327329991	2.89146329263680	0.18629773663510
F	-6.16668391666431	4.12380715944025	-0.96663161078096
C	-6.11767174873582	0.62536011868881	-0.06880925768327
F	-7.72591023003839	1.91754823703473	-1.20444050191016
C	-4.89629411653028	0.55470552701917	0.56531039075568
C	-4.09062765251274	1.68735602204417	0.70647499734285
N	-2.96117161992757	1.38433813702595	1.45814027567978
F	-3.80527864201155	4.00833875183903	0.30572245352854
F	-6.89397549129251	-0.45564612624852	-0.16660866273988
O	-4.40410770027424	-0.54472017533063	1.13582221561686
C	-1.82878742217744	2.21819990288750	1.38359975588728
C	-1.40305644229830	2.98952327405964	2.45660094088434
C	-0.26461973446216	3.77106621062924	2.38630052935255
F	-2.08498285844691	2.98285198650891	3.59520572580663
C	0.47992369110387	3.80012562993166	1.21890232969634
F	0.11272163949518	4.49689239725712	3.42947806370142
C	0.07801801516353	3.04515222908647	0.13000296407710
F	1.56937629758108	4.54699705630595	1.14764838872113
C	-1.06180508011498	2.26531373664215	0.22359017745762
F	0.78756008882081	3.06403109386280	-0.98848423124437
F	-1.41807602796327	1.53807857946329	-0.82519236916699
Si	-2.88495312996721	-0.33843419551787	1.96133607420786
O	-1.40499220130665	0.02590189863109	2.81739096627314
N	-1.98495201252212	-1.52804872755395	0.98590248777238
C	-0.39676868208835	-0.77854643051751	2.47838069722613
C	-0.67025298373958	-1.66227267159039	1.42306615740444
C	-2.56506103109090	-2.45782061192047	0.11605118598506
C	0.85106423395969	-0.75298712649313	3.06858296708639
F	1.10081654100480	0.06879048740192	4.08733667141646
C	1.85902033270831	-1.58190516848031	2.58990402282777
C	0.34735653358051	-2.46191406015478	0.93659974859185
C	1.60702554404991	-2.42508042428319	1.52378742893459
F	0.16139709599763	-3.26981890558927	-0.10993255841646
F	3.06510803005085	-1.55569236050668	3.14836260886065
F	2.57420404696733	-3.20396935183281	1.05120143087979
C	-3.10596099954558	-2.05973607911975	-1.10228657038830
C	-2.65725335955948	-3.80923476048745	0.43906597057944
C	-3.72217283172086	-2.95903257668707	-1.95568227142902
F	-3.03142950152801	-0.79264092822192	-1.47377168731838
C	-3.79475703404293	-4.29802434366178	-1.60926160415648
C	-3.25841736406543	-4.72441545789605	-0.40549233343884
F	-4.22532774822176	-2.54621326806116	-3.10907670857435
F	-4.36517257372348	-5.16957108043462	-2.42563266569929
F	-2.15534177125596	-4.24549669012873	1.58826261299192
F	-3.33058314007320	-6.00467243187925	-0.06617933581893
C	-3.62481231222944	-1.32454463185471	3.55136708997891
N	-5.29722206279458	0.16718157218159	5.22696465124427
C	-6.07123300868856	1.31994022314279	4.60210364223994
C	-4.50722281979840	0.53915494374252	6.47511645609891
C	-5.37612812503984	1.33671866120133	7.45683725762115
C	-3.25037201652206	1.32583696649326	6.09628235619513
C	-4.04860950003279	-0.71233825633026	7.22858647946252
C	-6.09775157364581	2.51592920635146	6.84025646234774
H	-4.72877063871725	1.65935075812436	8.27640069035911
H	-6.11513320812950	0.66208105612967	7.90186910476101
C	-6.91425748864323	2.04228078326183	5.65605772706092
C	-7.01123266953701	0.80410195772803	3.51599001473429
C	-5.12764479618085	2.30549788236737	3.91967994272731
H	-7.70890423999066	1.37523925339639	6.00701630133294
H	-7.41332083937822	2.88004142210866	5.16270677423372
H	-5.38650797955444	3.28659547083135	6.53417485910356
H	-6.74794855533704	2.98324763680914	7.58294107292010
C	-6.16757149858326	-0.98367583767915	5.48732292037836
H	-6.67214558917289	-1.27741280304415	4.57540826672964
H	-6.92247212160884	-0.77880529167561	6.25078259894262
H	-5.56706561783295	-1.82829239170730	5.80737974101784
H	-4.87646845347357	-1.25510149668005	7.68280034964636
H	-3.39628511801550	-0.38739853626411	8.03903606311400
H	-3.48291986100710	-1.40004527617409	6.60471787480467
H	-2.76122898143186	0.92008278851756	5.21227206493995
H	-2.53945643387668	1.27405337758417	6.92100774736758
H	-3.44214832441828	2.37694384041170	5.90986704008590
H	-4.34461818129612	1.79821587376424	3.36436940618620
H	-4.64914387070290	2.99895976251820	4.60188640603637
H	-5.69784404947496	2.90340924459621	3.20859211392484
H	-6.47470768503119	0.23985858959685	2.75521345495574
H	-7.45378647500331	1.66541794530373	3.01690668962787
H	-7.83178678672993	0.20205606437634	3.90336514387070
H	-4.35058337776641	-0.45378824668997	4.25169742161702
N	-4.44038931627067	-2.47698960460834	3.29085051214831
C	-2.60815778937752	-1.80801793271005	4.41426872226834
C	-5.63141078631391	-2.58928175897977	2.48039191868906
C	-3.95164268614721	-3.54698894321985	3.94678886765196
H	-6.09104953513452	-1.62224598367370	2.33874584664447
H	-6.33735927147235	-3.25225914862674	2.98182879128159
H	-5.40027868024184	-2.98973970681123	1.49246165540136
C	-2.79530490755689	-3.16152985374909	4.67446004962561
H	-1.81116343941641	-1.19231107272986	4.79697585327107
C	-4.42127613195400	-4.86937776135299	3.98146985224339
C	-2.09948179064502	-4.11035960148907	5.44960536773165
C	-2.56680708989829	-5.39520222714189	5.47952721696197
H	-1.21249700145184	-3.82105975616713	5.99936759195274
C	-3.71873291928753	-5.76533097755515	4.74623932717412
H	-2.05095076915957	-6.14823189516873	6.06106671469759
H	-4.04997073222989	-6.79596569391366	4.78374485745520
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[TS-a-FLP$^{C3\text{-}pos.}$]‡

C	-5.50732530099778	3.17909825098942	-0.43476100120805
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C	-4.29187062093781	3.04291522688015	0.23045713260447
F	-5.85387460815949	4.36447675200553	-0.92872410095639
C	-5.98682404157582	0.86055923612592	-0.06535609868715
F	-7.50534268133771	2.23229307324194	-1.23384675511141
C	-4.78559185729697	0.72853930149074	0.59450083797696
C	-3.92036516750318	1.81669108679417	0.75052751061144
N	-2.79068811716190	1.43195219135605	1.46426169658435
F	-3.51799601880770	4.12539516403436	0.34270402693269
F	-6.79651535279043	-0.19062528218314	-0.20847350991917
O	-4.35524772573313	-0.40371058927405	1.14803487471154
C	-1.69751586724828	2.30600036927704	1.60581491998837
C	-1.68744028107461	3.32161296686661	2.55163117272844
C	-0.57963891655672	4.12418786578976	2.75554807290509
F	-2.76684250900534	3.54233174457445	3.29555005095063
C	0.55995383199300	3.92278477078838	1.99579428671390
F	-0.60531057158689	5.07676896103497	3.67881794442702
C	0.57193298137397	2.93296913761915	1.02662880998978
F	1.63132520714983	4.67410081535156	2.19163893937754
C	-0.55165673057577	2.14938389371410	0.83338791656347
F	1.65917103912094	2.73843535349900	0.29541951711249
F	-0.50902889204771	1.20622789389336	-0.09604245154161
Si	-2.75151803640272	-0.32105621501240	1.86984652986473
O	-1.16748393619426	-0.10359053732171	2.56627928072511
N	-2.02803696576820	-1.55330460835052	0.77374334862313
C	-0.26090929378200	-0.97544528094593	2.12541201405643
C	-0.70554127197231	-1.83136593105281	1.10701788756804
C	-2.76652477162043	-2.35808454480446	-0.09277164918197
C	1.03311011459001	-1.04920024354560	2.59491700531180
F	1.45298926836334	-0.22504443066730	3.55597441148962
C	1.90793990469232	-1.99223760484968	2.06837736278587
C	0.18116658512190	-2.74732484581113	0.57236171983448
C	1.48056461411948	-2.83518986251643	1.06139270220052
F	-0.17045144154040	-3.56793006701404	-0.42204722787216
F	3.14952890795562	-2.08434993943914	2.53553789611290
F	2.31446084806712	-3.73684920568557	0.55010315796695
C	-3.39049924849021	-1.81078061627130	-1.21172461123062
C	-2.98375209754931	-3.71304947846364	0.14354541239061
C	-4.22671525269242	-2.55656566167606	-2.02407084846932
F	-3.19313095523247	-0.53763726074617	-1.51591844458548
C	-4.42981274909871	-3.90071431088501	-1.75590393493474
C	-3.79575793152168	-4.48150503033678	-0.67050768128260
F	-4.82837222431851	-1.99211348823923	-3.05963125310384
F	-5.22021494732884	-4.62685273845629	-2.53169552151611
F	-2.40472779069009	-4.30295828208362	1.18826318506516
F	-3.98669047564345	-5.76851452575948	-0.39841675506912
C	-3.42420353009552	-1.29778068825375	3.43239071482950
C	-2.47223520078605	-2.02661845484685	4.29558184291103
C	-4.30619927351419	-2.33521805722812	3.02111611552390
N	-3.99637103985319	-3.51188149957778	3.55381955504454
C	-4.68544343831100	-4.75724920037596	3.32524363980239
H	-4.00473902438640	-5.48290575712389	2.88025192836901
H	-5.51341998338877	-4.58432399795463	2.64159411540915
H	-5.07168825300967	-5.15345670760448	4.26555495628873
C	-2.86821963137478	-3.37017388268461	4.35600382987327
H	-5.13163302353141	-2.25379475891090	2.33091188846032
C	-1.33672561611008	-1.64598378579668	5.00649037206582
C	-2.19912977429741	-4.33864928152112	5.08874602243428

N	-5.14322964705896	0.00653802603584	5.18709203351605
C	-6.15378583308572	0.90560563733828	4.48616110891212
C	-4.41773770951896	0.65044420691601	6.35966415895034
C	-5.40847312699905	1.36404294816736	7.28890010499340
C	-3.33832215238100	1.60274912994000	5.84773717331975
C	-3.70856054309247	-0.39954257217362	7.21534383650021
C	-6.37963346120772	2.29407936094335	6.59272822312237
H	-4.82399393127590	1.90136652587483	8.04005181397214
H	-5.97951939890410	0.60577031286507	7.83572309808296
C	-7.10784564642104	1.53827482585689	5.49980098846318
C	-6.97507964014501	0.09739282780571	3.48229408349966
C	-5.44356107990336	1.99330294702768	3.68592531374625
H	-7.73339590765881	0.75972378557292	5.94947973827031
H	-7.78484573793559	2.19736822352596	4.95085329949031
H	-5.85578848759414	3.15971453773553	6.18107086356704
H	-7.09460982492650	2.69055822435998	7.31681199136161
C	-5.74410064735661	-1.26765824333316	5.58058395157834
H	-6.17779519719110	-1.75183245519927	4.71221913707904
H	-6.52456544794183	-1.15800132824549	6.33722959766374
H	-4.97231431900223	-1.92660124006916	5.96520805745798
H	-4.40386785484651	-1.04007023183256	7.75671107449890
H	-3.11869917645358	0.13165501953434	7.96241085598006
H	-3.02340694856009	-1.02054355131893	6.64167715419762
H	-2.74818336186005	1.13500285199109	5.05916778420039
H	-2.66259733041263	1.84462608837759	6.66835901992878
H	-3.72648338216479	2.53854494367829	5.46341426518612
H	-4.54187677725773	1.61707896889550	3.21296645605334
H	-5.16858330987502	2.85951852039782	4.27765193719428
H	-6.10794542034622	2.34680864902122	2.89794721954366
H	-6.34030449006260	-0.39971476260367	2.74954070193765
H	-7.60795763083992	0.79407729274755	2.93344282612752
H	-7.63628166551379	-0.62973395204220	3.95164231025250
H	-4.19821683714638	-0.49638258868810	4.19666649022440
C	-1.07802505144889	-3.92845774118178	5.78653299944746
H	-2.52592208696116	-5.37046978795354	5.10521044356987
C	-0.65370157436968	-2.59815159733136	5.74159443974887
H	-0.51577406968601	-4.64996846100003	6.36532177246050
H	-0.98113806291898	-0.62621461642525	4.96629012254033
H	0.23752959270313	-2.30797920391092	6.28352860478506

N-methylpyrrole

C	-5.16690116228945	0.54698176703580	0.02411218401416
C	-3.85986248128598	0.95099177922749	0.13581244639317
C	-3.87227158024094	2.35466360194824	0.31568418500583
H	-2.99439723257906	0.31069750700709	0.08146239990061
N	-5.96621199021669	1.64792930907479	0.12307553748696
H	-5.59425565214768	-0.43185108740837	-0.12175188136154
C	-5.18617564163889	2.75193969726134	0.30704993362420
H	-3.01792250880640	3.00263960073155	0.42673866332518
H	-5.62983878460678	3.72879262308001	0.41171123437400
C	-7.40414138130806	1.63324458338673	0.14583131931557
H	-7.78893556581091	1.58667633907913	1.16771513416335
H	-7.76676877320960	0.76552883999430	-0.40362053496051
H	-7.79360724585953	2.53031543958190	-0.33516062128099

[2b]$^-$

C	-5.58451507764461	2.18926910860980	-0.17438694334596
C	-6.21615978394706	1.02544859909731	-0.56091597825991
C	-4.29544936544457	2.15375875444345	0.34974037972605
F	-6.21253128173928	3.36185786853778	-0.30400366698657
C	-5.56209024497798	-0.19301521724436	-0.41812390622118
F	-7.45190408585253	1.07087963446979	-1.06693103176769
C	-4.28978218941589	-0.23452454598071	0.11474570636355
C	-3.63703952848794	0.94777888875632	0.50713087595588
N	-2.35962561890993	0.66514311599340	0.96157767792427
F	-3.72877803789829	3.32170918620912	0.68606200618560
F	-6.17655531999239	-1.31887617588391	-0.79558343950417
O	-3.58469243489721	-1.33840398190297	0.27760775553393
C	-1.59779790707576	1.63327494051682	1.61884370572938
C	-2.00508027519738	2.16904692308149	2.83713809768972
C	-1.22490362620944	3.06922970316998	3.53910577675662
F	-3.17225216781793	1.80520783241847	3.35396318261975
C	0.00603738198669	3.44646325159809	3.03233419597049
F	-1.64236218880157	3.56141279179254	4.70302322190251
C	0.43505256818107	2.93555898289607	1.81967946541629
F	0.77313599227710	4.29905376291502	3.70498373963179
C	-0.36668847864453	2.05000537345926	1.12128503085083
F	1.61403699535151	3.30917404956585	1.33109469652056
F	0.06957460713852	1.59708548423551	-0.04403804609718
Si	-2.01432491134581	-1.11699683399725	1.06886884529376
O	-0.35361670350971	-0.75835141196195	1.56200768206926
N	-1.27077983585707	-2.20779600774568	-0.17712319016535
C	0.55946167948821	-1.55009761277815	1.02825970446324
C	0.08044075704017	-2.42071548700298	0.03038387414145
C	-2.00705317488264	-2.94466709769413	-1.10552613273063
C	1.89620547305446	-1.54948212425952	1.37200054624476
F	2.36204583016878	-0.71161329654867	2.30280097634221
C	2.77457690935916	-2.43053194645482	0.75061875776788
C	0.96581558680506	-3.28830549831664	-0.58147742538249
C	2.30869396068894	-3.29762882788535	-0.21516482853626
F	0.57284620468183	-4.14472533077165	-1.53609876529323
F	4.06537301704971	-2.44299848723402	1.09443708845564
F	3.14895542537380	-4.15835367590564	-0.79874792391231
C	-2.56982449229573	-2.32140893927536	-2.21537101821529
C	-2.29599287767518	-4.29251240647148	-0.92207227883947
C	-3.40064694504915	-2.99709485264501	-3.09031783519067
F	-2.33520099178939	-1.03648967842401	-2.44027154299434
C	-3.66915948185390	-4.33847975595253	-2.88228893567523
C	-3.10725321425913	-4.99047238600711	-1.79864789491834
F	-3.94502023205154	-2.36816618464193	-4.12781170934989
F	-4.46316791555991	-4.99790613610616	-3.72015573492157
F	-1.80255006992780	-4.93401561083881	0.12908200664284
F	-3.36774650480476	-6.28009538674495	-1.59659114548300
C	-2.49199994087697	-1.95375550347791	2.64811695008339
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N	-3.67899012527066	-3.09897251407592	4.16024709839665
C	-4.72362170126142	-3.88940196524501	4.74790034854062
H	-4.56241385285088	-4.95879879331293	4.58356426079311
H	-5.67988642016449	-3.61039545043056	4.30679632024544
H	-4.77325286585062	-3.70474549763782	5.82173672118413
C	-2.45243888002056	-2.86184149740473	4.72210257786617
H	-4.58049372241512	-2.64556142446934	2.28893949224768
H	-0.69242188418205	-1.80780689224123	3.96553940214324
H	-2.22789639236015	-3.21059636033925	5.71788572264415

1$\cdots C_4H_4NCH_3^{C3\text{-}pos.}$

C	-5.82434386155275	1.60079025607012	-0.12073947584287
C	-6.38951793240485	0.37091867303021	-0.40924040458129
C	-4.51724055742355	1.68813739744735	0.34583784647981
F	-6.53209966474738	2.70827484134048	-0.30206340079448
C	-5.64947904104838	-0.78896931795197	-0.22363701614888
F	-7.63157251127731	0.29846262368314	-0.86993593813522
C	-4.36019384719851	-0.70268185202781	0.25568743672867
C	-3.77679755743147	0.53611212401857	0.54297670614478
N	-2.45741724335333	0.36715962262085	0.95314280298688
F	-4.00538537043952	2.89651583925335	0.57330952889130
F	-6.18463591569386	-1.97310693555804	-0.52354746033149
O	-3.55457833080733	-1.75829031244248	0.43073094645486
C	-1.71968439752544	1.39980138779787	1.54913971014324
C	-2.15622611079685	2.02539198647471	2.71072782891256
C	-1.40462548690257	3.00082593567070	3.33878444136073
F	-3.32244914479099	1.67051159180838	3.24450753368166
C	-0.16996583482217	3.35258291049013	2.81794873277308
F	-1.84728936444552	3.58329199003385	4.44224465230929
C	0.29695943009675	2.73244302635548	1.67006538634110
F	0.55950150578545	4.27651885260420	3.41808197998236
C	-0.48151020878930	1.77569097265888	1.04265320059673
F	1.48150304386917	3.05893463201985	1.17924438211596
F	-0.01584796171503	1.19202374006834	-0.05164072783920
Si	-2.00372258668270	-1.33396353806275	1.00615416084064
O	-0.52201281496169	-1.07083800335501	1.81635356963006
N	-1.16623485673120	-2.34710312619350	-0.16265034022132
C	0.51364529835698	-1.72381068008065	1.26469454668616
C	0.19009648838026	-2.47116804536662	0.12797164265856
C	-1.80660721996589	-3.14976794591153	-1.11580284600440
C	1.80992148601574	-1.65959653712026	1.72994146011740
F	2.11677880189709	-0.93201882395191	2.79820399752731
C	2.80691344061032	-2.35503475837869	1.05643382399462
C	1.18883267854602	-3.15647172115960	-0.53818399518967
C	2.49541900066319	-3.09965884856841	-0.06808115406378
F	0.93491783779409	-3.86933499759567	-1.63589509015269
F	4.05912536459880	-2.29860424133416	1.48976556272448
F	3.45128631736216	-3.75955888533347	-0.70987198774579
C	-2.47126290992997	-2.57803966333094	-2.19373765887120
C	-1.87678228240365	-4.53021354326343	-0.97520407034795
C	-3.19136526081644	-3.34574932030907	-3.09183654309918
F	-2.44920301842413	-1.26255169766154	-2.35526008205281
C	-3.24135523889290	-4.72135317847707	-2.93114855648409
C	-2.57490486542891	-5.31681193106417	-1.87220319057313
F	-3.83137609953607	-2.77204770078396	-4.09857430861637
F	-3.92784333487507	-5.46655394151233	-3.78025638728448
F	-1.27401594700634	-5.11781644761695	0.05436195383108

F	-2.62668896749680	-6.63085474033108	-1.71106680809703
C	-2.70098897365693	-1.82767401782849	3.28268673229402
C	-4.08278748215003	-1.86498568368303	3.28700105225343
N	-4.47589519928104	-3.06691663931280	2.80991555515219
C	-3.39216187071521	-3.82471537833632	2.49565049305606
C	-2.25929337035635	-3.10127179167119	2.78431977514929
C	-5.84407625574789	-3.43938407423015	2.52741637254067
H	-6.51214475050072	-2.81613405063418	3.11751406073012
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H	-6.06406209843490	-3.30148520389565	1.46920078433768
H	-2.08669977672585	-1.06213445699823	3.72720286815893
H	-4.79932552820178	-1.11430419482691	3.57663816419083
H	-3.50424212055230	-4.80909875944301	2.07269208185945
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[TS-b-FLP$^{C2\text{-}pos.}$]‡

C	-5.58659702306091	3.05225621854566	-0.44543520067860
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F	-5.94160744730573	4.23399319880598	-0.94180938079405
C	-6.03506359837542	0.71935517960676	-0.10712313061674
F	-7.52557923597643	2.06439109889923	-1.33818051314353
C	-4.86189180830434	0.60814869402797	0.60576568103718
C	-4.02733881854341	1.71239423408935	0.79611835067313
N	-2.92953065315116	1.36080692047540	1.57274776973249
F	-3.66381950892003	4.03267903588369	0.46739511639917
F	-6.82060408565877	-0.34511715320630	-0.28361718311144
O	-4.43897242681982	-0.51179262700112	1.19253879732204
C	-1.76374195238510	2.15241084547968	1.53849095669052
C	-1.37087202415174	2.93544971586349	2.61467705512209
C	-0.18059247366649	3.63940380145367	2.61055209932843
F	-2.13244095966077	2.99892549661102	3.70066605604193
C	0.65174320599238	3.57400070375673	1.50568153106010
F	0.16867379808672	4.37107798238643	3.65953494781497
C	0.28054297521581	2.81189213689121	0.41077337094825
F	1.79635741794301	4.23691662969569	1.49618364466340
C	-0.91431526864148	2.11362665484986	0.43761215074206
F	1.07429182990269	2.74658430697904	-0.64711337402982
F	-1.23743548465899	1.36790855489732	-0.60981768610543
Si	-2.89223849341598	-0.38700262054733	2.00214416711207
O	-1.36541463669689	-0.10019107199264	2.81500910252651
N	-2.04864819088957	-1.54398892164259	0.93642742550315
C	-0.34045857614258	-0.74910263354548	2.26101984203905
C	-0.68074837522713	-1.59492918180458	1.19550459399824
C	-2.64725011589030	-2.43619988249119	0.04160933342631
C	0.97790251756029	-0.58766968988074	2.63575054369311
F	1.30250145577800	0.24031676260296	3.62815855507178
C	1.97899681746410	-1.27906434648739	1.96176970816287
C	0.32287466897355	-2.26599050027324	0.52253273524433
C	1.64931891448927	-2.11668809803150	0.91344909104311
F	0.05819949583991	-3.05434831673306	-0.52345969493312
F	3.25004314757069	-1.12957489616392	2.32170348536604
F	2.60282040637676	-2.77744488843490	0.26410378305669
C	-3.22518057219613	-2.00112515019137	-1.14674900719351
C	-2.69766327575260	-3.80195289994247	0.30708897834815
C	-3.83964590107681	-2.88064508417742	-2.02234314190081
F	-3.18214289664298	-0.72046288103643	-1.47230645537833
C	-3.86721717556880	-4.23509397526615	-1.73377477840462
C	-3.29225099549286	-4.69811311216888	-0.56188746500505
F	-4.38080932200259	-2.43510545379783	-3.14520583346287
F	-4.43149964887178	-5.08519016400184	-2.57624681272247
F	-2.15596809184788	-4.27160502165990	1.42590889667903
F	-3.32061724713406	-5.99339720440665	-0.27561340967651
C	-3.61490784258113	-1.36137548392363	3.56370550988561
N	-5.33181945514907	0.07874967805572	5.23848790902669
C	-6.11985659102832	1.21192251873364	4.59150886615269
C	-4.57514269992075	0.47823962361541	6.50034459465790
C	-5.48431169107105	1.25727787898586	7.45983857755968
C	-3.33025766576999	1.29094279872237	6.13811540706977
C	-4.09744811564177	-0.75622280909367	7.26923135491202
C	-6.23682197142994	2.40746697359607	6.82447638243877
H	-4.85986885164315	1.60794975340584	8.28557537870257
H	-6.20667231810679	0.56272520466617	7.90180824820471
C	-7.01193979631382	1.90480644811868	5.62346599279420
C	-7.00474405175243	0.66645330434997	3.47361594929375
C	-5.18744971276239	2.22923969520980	3.94088281732436
H	-7.79293373412036	1.21342759293863	5.95713109049990
H	-7.52609143527121	2.72581979843194	5.11780941386642
H	-5.54909160317654	3.20405286513624	6.53199889892087
H	-6.91868453273690	2.85077806432959	7.55330359473743
C	-6.18848101547393	-1.08458304722526	5.49580023398081
H	-6.66427466770659	-1.40089856347983	4.57577286178360
H	-6.96734033338236	-0.88194978671079	6.23445252790466
H	-5.57988338029577	-1.91117949351636	5.84488472256852
H	-4.91852957966866	-1.31955941522195	7.71088961341299
H	-3.47152034841781	-0.40894793879687	8.09108287104931
H	-3.49977549110587	-1.42886640620775	6.65866668673541
H	-2.81849493203419	0.88678764328946	5.26620868719526
H	-2.63298294840790	1.26024277851119	6.97533603737271
H	-3.54102209556154	2.33571260588196	5.93914325379698
H	-4.37009480799456	1.75090922676817	3.41002050665225
H	-4.75523623504145	2.93861649586446	4.63746684043361
H	-5.75519942977265	2.80794293819751	3.21235942441201
H	-6.42020737274916	0.12060150850233	2.73396494068786
H	-7.45565788617793	1.51318206143361	2.95747930833257
H	-7.82051993448515	0.04066742954553	3.83305376642150
H	-4.39639844002171	-0.52027411155726	4.29857231466603
N	-4.38623921150899	-2.53915192132597	3.28395710171140
C	-2.60818480308004	-1.85368118971201	4.45257592160952
C	-5.52905679663236	-2.69731144532376	2.40342164064184
C	-3.89223771088633	-3.57912800473235	3.94550142044779
H	-5.21462148298472	-2.77874697024750	1.36592316843890
H	-6.19878265363852	-1.84847042136521	2.47729346098159
H	-6.05891412534831	-3.60117023821320	2.69978344798334
C	-2.78184642138911	-3.19630857658033	4.69352243638943
H	-1.82433088799086	-1.23142118274497	4.85154517842161
H	-4.35191883414719	-4.55248208856317	3.85708442216837
H	-2.18587264832446	-3.84197656103252	5.31762316985619

[TS-b-FLP$^{C3\text{-}pos.}$]‡

C	-5.55327307874353	3.07040420873030	-0.45586734193052
C	-6.37113348246728	1.97264262810559	-0.65679156874501
C	-4.37487606712755	2.94740953736314	0.27415050949247
F	-5.89846518273061	4.25471406718823	-0.95374067291445
C	-6.01784755922515	0.73999879908262	-0.12051132951546
F	-7.49324452530810	2.09461076024550	-1.35971486537705
C	-4.84808719332127	0.62008464878300	0.59748174208667
C	-4.00710616052773	1.71938773725075	0.79031469914772
N	-2.91622344246877	1.36704135373754	1.57769023057152
F	-3.63095763766335	4.03903756322404	0.47005356975450
F	-6.80912650796735	-0.31859021304123	-0.30273909266323
O	-4.43882111609225	-0.50177910167707	1.18956062509528
C	-1.74506264921158	2.14942988700121	1.54151480401450
C	-1.35442116948546	2.94110029043376	2.61228585049257
C	-0.16454474521780	3.64601269383047	2.60328771456245
F	-2.12281483718377	3.02071337713944	3.69135324098248
C	0.66734594493940	3.57486908076647	1.49836420223692
F	0.18275867131217	4.38876781621351	3.64499025553650
C	0.29732536521281	2.80541214999074	0.40837153606182
F	1.81003951958698	4.24133328212332	1.48378132558117
C	-0.89589327671146	2.10452660962739	0.44031952960912
F	1.08929250047711	2.73745362407346	-0.65091809246347
F	-1.22046452806941	1.35765517116407	-0.60546845672511
Si	-2.89134641722009	-0.37282188949103	2.02057656634564
O	-1.39285378716514	-0.11468108828957	2.89730225363515
N	-2.00954351320988	-1.48989615848496	0.93967673605451
C	-0.34839334831785	-0.73622359938814	2.34877082135997
C	-0.65096032004042	-1.54269741699714	1.24109860810188
C	-2.59265782124904	-2.40380299880145	0.05893372894599
C	0.95652107904628	-0.59667024946847	2.77683750236680
F	1.24895138622615	0.17930753392645	3.82022286350614
C	1.97919870921790	-1.26340904981722	2.11013533653576
C	0.37399275337502	-2.19030814605258	0.57756095367957
C	1.68668463850583	-2.05845711120795	1.01807155893584
F	0.13918726018761	-2.94223696085066	-0.50253358192128
F	3.23672793220080	-1.13178777178337	2.52169677384236
F	2.66260305788119	-2.69582156253926	0.37755316452999
C	-3.17409948792117	-1.99795044804293	-1.13855571404739
C	-2.63465769107846	-3.76480849582337	0.34795507291513
C	-3.77689841464376	-2.89941580830930	-2.00014646331318
F	-3.14493184190691	-0.72401364416722	-1.48742563131272
C	-3.79966510329641	-4.24778382867058	-1.68420725211716
C	-3.22495950167428	-4.68117075497708	-0.50170245112561
F	-4.31429776742364	-2.48009457970799	-3.13489142848660
F	-4.36112988313387	-5.11909812711114	-2.50709848225681
F	-2.08741192944857	-4.21484822285733	1.47521652323643
F	-3.25192074935371	-5.97083302031491	-0.18188326181502
C	-3.64507885424637	-1.37852816070249	3.51918418403898
C	-2.69938196681555	-2.09971378591715	4.36527141902342
C	-4.51887823827855	-2.40960613845690	3.07464661594839
N	-4.16026174239666	-3.57859115200927	3.59146468787385
C	-4.77735310385650	-4.85504059420872	3.31375851231708
H	-4.06551673058144	-5.51033843331409	2.81154339811466
H	-5.63623391798560	-4.70014889653821	2.66496897039657

H	-5.10832158691228	-5.32392332723813	4.24059452457574
C	-3.04001275342729	-3.40590804159305	4.39388276164969
H	-5.34207087327420	-2.33671544294677	2.38204738947887
H	-1.84925537764519	-1.65702412828548	4.85695968057212
H	-2.58533737982962	-4.25328725211814	4.88108223858429
N	-5.28280969282284	0.04933273508263	5.24267801263082
C	-6.12960243387191	1.13083537626528	4.59079846389274
C	-4.51390572713720	0.49138780263668	6.47611857802081
C	-5.42898950275699	1.25117734242789	7.44442809756315
C	-3.30312081727174	1.33135806984696	6.07350022437818
C	-3.96959174645618	-0.71552578462944	7.24390172806390
C	-6.23626597432085	2.36261926182898	6.80562183758812
H	-4.80442654316186	1.63745223895565	8.25396406182031
H	-6.11745710732121	0.53603724582486	7.90770995707242
C	-7.02134785029087	1.81311065767350	5.63065270732580
C	-7.02023047264283	0.51152803769151	3.51319355001466
C	-5.25593070744752	2.17243332891892	3.89402801171543
H	-7.76883827610159	1.10009294303119	5.99492418401581
H	-7.57634489698574	2.60708152674906	5.12469505040176
H	-5.58272461640211	3.17713274250461	6.48494045447704
H	-6.91717936006978	2.79532997658267	7.54180982118246
C	-6.07217869873244	-1.15106037136106	5.51145215131765
H	-6.52501103831851	-1.50393632288008	4.59078313171545
H	-6.86769904277660	-0.98693278912664	6.24278603155058
H	-5.42233688062410	-1.94149653132609	5.87291235930324
H	-4.75514258434297	-1.30206339605235	7.71930142236363
H	-3.32614513489831	-0.34016817327049	8.03948288451255
H	-3.37131991331529	-1.37174993598561	6.61501359995003
H	-3.55377050163670	2.34001108435632	5.76728805624202
H	-2.74461782082843	0.86557467717457	5.26148034027869
H	-2.63439747900187	1.41328782594359	6.93055216318264
H	-5.85032500026951	2.68113913730323	3.13552455018885
H	-4.40174634622766	1.72485429848507	3.39502075085000
H	-4.87711233053529	2.93873711542575	4.56271925258998
H	-7.82169713558452	-0.10057243845329	3.92568820143124
H	-6.44587755806844	-0.08037655102756	2.79938805338172
H	-7.49099767887443	1.32048731155590	2.95606191094529
H	-4.34851168721702	-0.53168946095279	4.24170240497168

[TS-b-ELC-O$^{C2\text{-}pos.}$]‡

C	-5.64827034781059	1.48862056587355	-0.21752251838743
C	-6.28649101507822	0.27162368309806	-0.37361207904797
C	-4.35259428924595	1.55680311338673	0.28242742049288
F	-6.27406955727009	2.60776058647107	-0.55074960335777
C	-5.62125788836318	-0.89576009818492	-0.02449867860628
F	-7.51897803195671	0.21769444186654	-0.85808559374697
C	-4.34190762608973	-0.82126812128875	0.48174626903911
C	-3.68310318178636	0.39973352269368	0.64790356857971
N	-2.38237801178426	0.25313793635442	1.12298732413310
F	-3.78858002226424	2.75916581837571	0.38500496097554
F	-6.21482885544185	-2.06971993151877	-0.19201792724720
O	-3.58659919518879	-1.90745634343575	0.78070558764093
C	-1.59667794005806	1.37415182986998	1.44880341238407
C	-1.88653588894133	2.15533520475292	2.55945350733444
C	-1.09813409472660	3.23335174317224	2.91543057064260
F	-2.95357800394542	1.86935046982559	3.29906078472112
C	0.02331909544184	3.53614435972539	2.15954467656047
F	-1.40406691368051	3.96897385014723	3.97291608405968
C	0.33644002742737	2.77147973749228	1.04730680843567
F	0.79345846245372	4.55427349062274	2.49912421610177
C	-0.47679561953455	1.70788208814014	0.69842512869262
F	1.40486792726362	3.06519267040044	0.32423421053592
F	-0.16145004575703	0.98614161360345	-0.36787475056202
Si	-1.80186354772652	-1.39582883395990	1.36638726062206
O	-0.23858271280490	-1.00690477673362	1.93076585731056
N	-1.08886393436717	-2.42865833681334	0.11989255196024
C	0.74562343388513	-1.53718985232855	1.18985043516414
C	0.31054019299325	-2.37108310663377	0.15342910671269
C	-1.77450365948957	-3.12377949966534	-0.89006329977958
C	2.08555062157113	-1.27286408410555	1.37857750643534
F	2.48858476547590	-0.44352664368089	2.33451909938835
C	3.02201582818414	-1.86654071944964	0.54113379334412
C	1.25059416235692	-2.95642966423393	-0.67470101772729
C	2.60429154760314	-2.70569704120136	-0.47454405019221
F	0.90205803718209	-3.75620403318872	-1.68315717328578
F	4.31473274543734	-1.62570521098307	0.71587218243118
F	3.50088150559471	-3.27244332186537	-1.27267547782868
C	-2.50709162036217	-2.43909570398088	-1.85191145547545
C	-1.80465722480633	-4.51193069034866	-0.93788173657655
C	-3.28378153499424	-3.10019753996116	-2.78615912892557
F	-2.49567572002853	-1.11303577339234	-1.86315642316204
C	-3.30322587127988	-4.48491132503019	-2.80267943483879
C	-2.54888364092597	-5.19434216319168	-1.88223118612342
F	-4.00938670030391	-2.41581762483495	-3.65517613855065
F	-4.03787786192277	-5.12862512763293	-3.69148695520416
F	-1.10460663438925	-5.21696974790809	-0.05496369943930
F	-2.55623365487178	-6.51816203575973	-1.89958030942340
C	-2.54209859592829	-2.16528211183221	2.95469341196727
H	-3.49256197986416	-2.28866890107809	1.95891981518088
C	-3.25823729962173	-1.40898674700041	3.91149710825254
C	-3.19615496691196	-2.06399973603682	5.13317658009876
C	-2.42724599219217	-3.20192611003338	4.92933103696751
N	-2.03897678332500	-3.26115301325038	3.65160650604097
C	-1.18226004970097	-4.27753461719869	3.08693373924706
H	-3.65442655339692	-1.76777058086465	6.06216017545944
H	-2.14968411464793	-3.97904572773031	5.62537538137205
H	-3.77254024434161	-0.48476992167671	3.69744414523890
H	-0.98856559326340	-5.03558154587138	3.84235680924517
H	-1.65802297617243	-4.74552592540020	2.22801458703338
H	-0.23344235630720	-3.84317443658702	2.76981701768626

[TS-b-ELC-O$^{C3\text{-}pos.}$]‡

C	-5.72346953770442	1.62875966193033	-0.42062593144435
C	-6.34323867899413	0.41728952432974	-0.66504922718812
C	-4.46480597098840	1.68079754694604	0.16946003805296
F	-6.33096804451688	2.75959832537835	-0.75087505366031
C	-5.69399499705400	-0.76161439651742	-0.32079214873491
F	-7.54607044390964	0.37968656673087	-1.22279248813650
C	-4.45350754756732	-0.70315595893123	0.27563524311714
C	-3.81853960961970	0.51270278679596	0.53744443619129
N	-2.55786466464428	0.34805131612256	1.10825404469871
F	-3.91632221608757	2.88017016227722	0.35871390151695
F	-6.26728174531645	-1.93129312220740	-0.57433105860245
O	-3.72141928590729	-1.79470340504169	0.59871437776545
C	-1.78061172621379	1.46112897254761	1.48086820359763
C	-2.07886376670977	2.19357724636236	2.62129933089576
C	-1.29103347348660	3.25384371525398	3.02941869390673
F	-3.14717508984569	1.87128691680590	3.34498181071251
C	-0.16378741058676	3.58610944802635	2.29493033786176
F	-1.60203009834000	3.94398721076369	4.11643189150411
C	0.15701171993452	2.86944431323210	1.15309823787202
F	0.60713834336126	4.58586787523570	2.68422758873805
C	-0.65488997305412	1.82353725702945	0.75345908426007
F	1.23430408631060	3.18881876551351	0.45418866208868
F	-0.32874880680542	1.14022494456821	-0.33413269725043
Si	-1.97353982149268	-1.30350638994756	1.31389863876595
O	-0.44630272241182	-0.86774817380421	1.94478108771295
N	-1.18880851946279	-2.34880568872787	0.13066802237351
C	0.57471012441979	-1.47427609255710	1.32571939728848
C	0.20206146053265	-2.33676289450838	0.28806431495957
C	-1.81151310368936	-3.12773956329039	-0.85468870554083
C	1.90276437972097	-1.25958184846466	1.62855544378510
F	2.25189114747885	-0.40942434492977	2.58816812814006
C	2.88511601804158	-1.93078496898173	0.90966958325543
C	1.18636818239289	-2.99186774300497	-0.42736684988333
C	2.52542951021325	-2.79436736140991	-0.10791775826110
F	0.89527198912974	-3.81470258168345	-1.43685936170656
F	4.16665962536190	-1.74086926500035	1.19918997559705
F	3.46218813157718	-3.44090108473423	-0.79225306906373
C	-2.44667017483826	-2.53399262497226	-1.93803795695782
C	-1.86783277224489	-4.51197198628855	-0.75769972466528
C	-3.12916730021570	-3.28305139698866	-2.88017300917298
F	-2.42783083073188	-1.21483383094117	-2.06551704299547
C	-3.16330224914540	-4.66304440282965	-2.76170800126228
C	-2.52384764023124	-5.28200877167555	-1.69916797212889
F	-3.74771819242993	-2.68860250837804	-3.88795964282820
F	-3.80783077699433	-5.39052178103895	-3.65665891302382
F	-1.28182498751377	-5.12096304707597	0.27161707763544
F	-2.55654262333284	-6.60124375687806	-1.58427651666174
C	-2.74948934474253	-2.20495747320895	2.80874589266225
C	-2.49394137555263	-3.54132265479046	3.15204502676945
N	-2.78673912707918	-3.72829306770424	4.44123922197020
C	-3.22589367854665	-2.54077868285281	4.99442707862087
C	-3.21233917457786	-1.58766048006979	4.02833010979927
C	-2.69974712274966	-4.98208710011439	5.15519797004286
H	-2.04818104018228	-4.87476806171261	6.02207037684703
H	-2.28729685944555	-5.73995999396361	4.49354146954623
H	-3.68877820408174	-5.29888130076091	5.48692650513877
H	-2.13112746604221	-4.35023170175493	2.53607586967820
H	-3.51334103975387	-2.49602046007566	6.03223781186935
H	-3.49779103555970	-0.55455571869548	4.14597495417367
H	-3.65961744807413	-2.16001486933687	1.80658188475756

[TS-b-ELC-N$^{C2\text{-}pos.}$]‡

C	-5.85507644015514	2.11255461974060	0.07807010443857
C	-6.10839885270802	1.12534054191345	-0.86014445089608
C	-4.73835842509936	2.02715831946334	0.90018327385436
F	-6.69168684967987	3.13265880369529	0.20695914564068
C	-5.23710584707001	0.05108048653442	-0.99343390281510
F	-7.18886603043786	1.19706696777483	-1.62244094235299
C	-4.12449480092552	-0.02304022887334	-0.18091711635162
C	-3.86389274545637	0.96213937790311	0.77275419763249
N	-2.71068674962971	0.67649103815255	1.51798204144803
F	-4.53848613551216	2.97899048884573	1.80678843419312
F	-5.48136932579644	-0.89246304623469	-1.89401656870070
O	-3.23480968747981	-1.02619641710279	-0.26518071572696
C	-1.90354835232431	1.73694355385078	1.97952676765759
C	-1.83218741924532	2.04004050137003	3.33154287974262
C	-0.96728286268242	3.00738587828742	3.81268032150014
F	-2.60714155472783	1.39005953958787	4.19348026641253
C	-0.15261375318227	3.69563770905825	2.92937549171684
F	-0.91825251908959	3.27748683159297	5.10795576133167
C	-0.21609206883524	3.42066917994559	1.57149009651227
F	0.68444003713802	4.61242305900852	3.38203608355016
C	-1.08923461167461	2.45247087020806	1.11078900491573
F	0.56811599200636	4.07275924751891	0.72976720169094
F	-1.13082713612526	2.18618011778852	-0.18702666764449
Si	-1.97567565144812	-1.09326670022364	0.85430596380501
O	-0.43973614100199	-0.45220399527855	1.12007509385984
N	-1.23133594529594	-2.51175323746525	0.06239110902914
C	0.56761896495491	-1.27937626028326	0.76318252755145
C	0.15029909392325	-2.46942106906060	0.15978286933406
C	-1.88516488156710	-3.43140676700977	-0.76797794741543
C	1.90230145433014	-0.98974988063758	0.93606505679769
F	2.28564512949314	0.15661427607648	1.48758414568075
C	2.85527102587676	-1.91135986974150	0.51519850039609
C	1.10464857168338	-3.38750898560380	-0.23948011666026
C	2.45406470096657	-3.10167692663862	-0.06660887813099
F	0.76140331418176	-4.55268559055383	-0.79210268898674
F	4.14700572987854	-1.65268840804916	0.67993314349316
F	3.36372585113531	-3.98499264893431	-0.45909705406140
C	-1.91897438411195	-3.24841672474439	-2.14692559871006
C	-2.56143177259272	-4.52829180573481	-0.24921594287086
C	-2.60037810876987	-4.11770115231140	-2.97907678017289
F	-1.28985289863750	-2.21452094031654	-2.68257279959683
C	-3.27327197854762	-5.20012799333812	-2.43386236744277
C	-3.25721003134686	-5.40526335750973	-1.06427592051568
F	-2.62392227171759	-3.91729069285554	-4.28669471422649
F	-3.92879009995213	-6.03521920598488	-3.22104614394748
F	-2.54943588844170	-4.75667377325498	1.06074683645249
F	-3.89920475769304	-6.44051764248014	-0.54070492138793
C	-2.65311906980417	-1.66477884859893	2.55691944060903
N	-3.75677514986042	-2.49660310967166	2.77409223626186
C	-3.59124271966914	-3.17446364374360	3.91089743169440
C	-2.37461435633944	-2.83008946282013	4.49221855610205
C	-1.78846274470204	-1.89967936523035	3.65339714221673
H	-2.91660455465827	-0.36281459995513	2.43157311937957
C	-4.91558010120290	-2.59959113623671	1.91649148367020
H	-4.62185821778386	-2.88520206808977	0.90771907721164
H	-5.44525115137093	-1.64745749707572	1.87265914592144
H	-5.58304558850335	-3.35762114713855	2.31898166854447
H	-0.83667749010660	-1.40908820963645	3.78905421895277
H	-1.98746673840507	-3.21717719374575	5.42028201676501
H	-4.34991500420038	-3.85890180615264	4.25913038264699

[TS-b-ELC-N$^{C3\text{-}pos.}$]‡

C	-5.90048756063603	1.95169162163851	0.30288809456168
C	-6.16145185141667	0.93754456160066	-0.60453570047303
C	-4.72311599828832	1.94488555429631	1.03726583117826
F	-6.78810577535711	2.91998202435520	0.48423225882116
C	-5.23580800131000	-0.07984411744866	-0.79688530811992
F	-7.30278205114165	0.93224508201806	-1.27775091748681
C	-4.05759517526762	-0.07270678355922	-0.07522438499048
C	-3.79123693154500	0.93801761476211	0.85094738314259
N	-2.57875394955703	0.73287093919011	1.52167779706661
F	-4.51087119603367	2.92171332901865	1.91425342043651
F	-5.49111820642498	-1.05062172153339	-1.66540696826005
O	-3.11390009891286	-1.01771807879848	-0.22765543699415
C	-1.78781590078221	1.82914252664697	1.90661059471228
C	-1.17590956896924	1.83056835131471	3.15361102028679
C	-0.33395805088137	2.84622724575220	3.56175704873288
F	-1.39181204507293	0.81392023509702	3.98503415149341
C	-0.09064896459579	3.91308196709107	2.71415855363192
F	0.23094088140620	2.80367839159418	4.75855765315293
C	-0.69412720524288	3.94666079074709	1.46799071974476
F	0.71452863534614	4.89061351236415	3.09226585892238
C	-1.51897819724285	2.90812293787955	1.07096706287359
F	-0.46761838105493	4.96694711154809	0.65588504727513
F	-2.04913924602407	2.95049474845806	-0.14627761010660
Si	-1.84499839487167	-1.06003620411832	0.88365120996143
O	-0.31796964516424	-0.38576996409205	1.10766735187194
N	-1.08182040428398	-2.48975229198120	0.13386873860712
C	0.70172106347721	-1.20309068892027	0.76015333119731
C	0.29888894950506	-2.41984779333567	0.20024125302585
C	-1.75991676844726	-3.48434490925036	-0.58081902691163
C	2.03312108566853	-0.88750293617460	0.91295983802300
F	2.40481283984001	0.27919755606742	1.42819002757214
C	2.99714219643491	-1.80826054629645	0.51470153934241
C	1.26422884078090	-3.33369854150774	-0.18078322396644
C	2.61018435273621	-3.02232362719879	-0.02557967310455
F	0.93469750074444	-4.52065646755964	-0.69519181037667
F	4.28661859195003	-1.52568379785186	0.66155740750979
F	3.53079104470675	-3.90514311251586	-0.39383639537598
C	-1.85701730069254	-3.42568228909137	-1.96757354828187
C	-2.42173936977172	-4.52205688917382	0.06374669190593
C	-2.59856892792754	-4.34747562881137	-2.68377494512342
F	-1.23446370841611	-2.45836238281311	-2.62166658417651
C	-3.27600427926360	-5.35278261955035	-2.01126156930011
C	-3.18511793881206	-5.44267998505468	-0.63298367812914
F	-2.68053737473760	-4.26871516823766	-4.00186268991522
F	-4.00723706505359	-6.22267217528755	-2.68637475827516
F	-2.33462898874029	-4.65024820055174	1.38392393706438
F	-3.82435840217335	-6.40900765894803	0.01491290020721
C	-2.60311989118281	-1.64685507139910	2.53187818055875
C	-3.84434709646481	-2.30767836260581	2.56591306631991
N	-3.87949095954714	-3.12597126142094	3.61692939112218
C	-2.68109276907503	-3.04925545386510	4.30421200786628
C	-1.87880262138414	-2.16087808847806	3.66971840713443
C	-4.96942987833722	-4.00560941802175	3.97105631759533
H	-4.65576253854179	-5.04551033781539	3.87682158761719
H	-5.80541568174715	-3.82603616006525	3.29939405107107
H	-5.28928018314802	-3.81636480428563	4.99552422291122
H	-2.74368899891878	-0.32792621097291	2.43816725666057
H	-4.67897940595563	-2.23829912591031	1.88524540799512
H	-2.52432824038914	-3.64141723931820	5.19098298471308
H	-0.88382479379177	-1.87391998761930	3.96752462548107

thiophene

C	-5.46805537923536	1.19517833053200	0.00006434128883
C	-4.75356726650398	0.03317723877908	-0.00005083333486
C	-3.35450542049650	0.25853160583869	-0.00005034495879
H	-5.21089919448109	-0.94647083426280	-0.00002865068218
S	-4.44280182723024	2.55755205107475	-0.00029171872275
H	-6.53924091467948	1.31956029941388	0.00016072251263
C	-3.04097921903709	1.58589441576483	0.00006480938029
H	-2.06284632844282	2.04002739895573	0.00016018449941
H	-2.61260444989341	-0.52795050609617	-0.00002850998258

[2e]$^{-}$

C	-5.52395936328936	2.31120996146749	-0.22919043188293
C	-6.17001176184113	1.16434961643696	-0.64369941567997
C	-4.24314323541606	2.24546099772304	0.31046270264376
F	-6.12919748953310	3.49597647062503	-0.34854095541033
C	-5.53813408737629	-0.06787919978819	-0.51879686997504
F	-7.39823480030852	1.24052174368185	-1.16186082353977
C	-4.27250009790099	-0.13681072126036	0.02623550727559
C	-3.60878244017331	1.02507958965549	0.45270397510522
N	-2.34184822422625	0.71337727419670	0.92236811518702
F	-3.65999754438263	3.39579513291046	0.67607912677728
F	-6.16544544528637	-1.17342646540674	-0.92454459963707
O	-3.57954265998649	-1.25445342373983	0.17448538530520
C	-1.58635809314926	1.65519899981066	1.62596174863652
C	-2.00968802677863	2.14716298392226	2.85701674632117
C	-1.24282322418140	3.03057545649452	3.59467954951837
F	-3.17856154018306	1.75822466616362	3.35008641574677
C	-0.00879232778148	3.43099625035646	3.11340996791750
F	-1.67685306198369	3.48716668512202	4.76619838735743
C	0.43599836322943	2.96204240865160	1.88931103644760
F	0.74580066352367	4.26419859154779	3.82276210805326
C	-0.35258391584576	2.09334810115460	1.15563157468676
F	1.61528238461177	3.36036648147331	1.42254123994705
F	0.09803725414068	1.67695647391319	-0.01796505145502
Si	-2.01772403477933	-1.06819280491896	0.96967140528678
O	-0.37241277185315	-0.74680116579426	1.50989157731033
N	-1.27178756653637	-2.16862397711476	-0.26301260006543
C	0.54154672551034	-1.55216205867099	0.99310295978399
C	0.07250845686103	-2.40444981479629	-0.02256439905950

C	-2.01385732242296	-2.96896917599619	-1.13512005169120
C	1.86782328648781	-1.57560489755105	1.37319943470972
F	2.32018604885764	-0.75480413592501	2.32430297543077
C	2.74689205245646	-2.46626314141238	0.76784685122615
C	0.96157832242781	-3.27492676771118	-0.62596918508964
C	2.29266119542139	-3.31250870629012	-0.22203219021707
F	0.58427722815472	-4.10762308627197	-1.60534435812325
F	4.02496402105492	-2.50984024058602	1.15027323357804
F	3.13367568440626	-4.17891046966192	-0.79372889302718
C	-2.63810060224861	-2.41098607520860	-2.24699467089279
C	-2.22940442645663	-4.32299400917718	-0.90091124448112
C	-3.46196090296149	-3.15470407008103	-3.07220466973952
F	-2.46463675864634	-1.12702720558411	-2.52754182475913
C	-3.65648529402083	-4.50085248630174	-2.81531829832220
C	-3.03093082747134	-5.08784555525821	-1.72940194336302
F	-4.06636289493858	-2.58595657824103	-4.11056939506600
F	-4.43814494210859	-5.22774985271963	-3.60779602020864
F	-1.66078875087777	-4.90879369565201	0.14486832637931
F	-3.21793615695351	-6.38068541038746	-1.47951387000605
C	-2.53095779714812	-1.93400363744066	2.54076563803300
C	-1.78900645437335	-2.17898876682481	3.67242953685310
S	-4.10153013285523	-2.59995923279184	2.73359704604682
C	-3.76753792563367	-3.18860785938598	4.29472371323046
C	-2.48788768995091	-2.89152018858857	4.67327026972056
H	-4.51697003528892	-3.72479341730793	4.85673985248306
H	-2.06461844954035	-3.17436362869636	5.62825810556605
H	-0.76499259245391	-1.84502596276358	3.76853724912717

[1—$C_4H_3S^{C3\text{-}pos.}$]$^-$

C	-5.56449642056790	2.22881785237900	-0.17567535890767
C	-6.20041008796995	1.08058427812473	-0.60106663543035
C	-4.28284062098280	2.16890392207462	0.36337069877579
F	-6.18039126439609	3.40951194222504	-0.28101720880919
C	-5.55594171256658	-0.14637770810624	-0.48790140252908
F	-7.43033706958966	1.14910213612026	-1.11661321548142
C	-4.28848768908308	-0.21069888090927	0.05387391242842
C	-3.63592292510993	0.95365767426229	0.49346091076917
N	-2.36908425912367	0.64733156437873	0.96325404873054
F	-3.71224362890627	3.32138778610618	0.74162537432122
F	-6.17477100591545	-1.25605381875472	-0.90057710484255
O	-3.58685763464079	-1.32353522414355	0.18777323661617
C	-1.60918893128251	1.59409624430822	1.65465610348022
C	-2.02549524122288	2.09791479312345	2.88325691445648
C	-1.25028196477624	2.98032077818874	3.61307727781762
F	-3.19532855872568	1.71925732131596	3.38256365724913
C	-0.01503415355006	3.36906944137499	3.12522032693539
F	-1.67711738885435	3.44601984443311	4.78370809193365
C	0.42315016933160	2.88840132289625	1.90328744787079
F	0.74740784642641	4.20218232241092	3.82623216500535
C	-0.37382165736553	2.02056828919047	1.17781033192431
F	1.60502719913845	3.27290103433525	1.43192285855688
F	0.07213838135432	1.59017044869570	0.00731878598337
Si	-2.04526430517043	-1.13798881808640	1.03045536815884
O	-0.39646587230608	-0.80707677027627	1.57363097045599
N	-1.28731406039205	-2.25348535735035	-0.17574614278464
C	0.53868505281312	-1.55421043571962	1.01125283189302
C	0.07337460761592	-2.42573422246065	0.01017440306665
C	-2.00374180887485	-2.99834289672772	-1.11595634880416
C	1.88122635211741	-1.50182537982816	1.32673901959016
F	2.33279965777876	-0.65483882754841	2.25560645949329
C	2.78046610098707	-2.33726817035666	0.67306098137562
C	0.97734409744644	-3.25280100907353	-0.62996243653651
C	2.32731629061422	-3.21159691396089	-0.29284658206346
F	0.59648218212357	-4.11404005724253	-1.58412545188642
F	4.07831116304719	-2.29916320297400	0.98534492534522
F	3.18774618739269	-4.02899248157765	-0.90642540373576
C	-2.52379938584213	-2.39407716156742	-2.25537265658477
C	-2.30183935922418	-4.34126362887823	-0.91562895901654
C	-3.32449652399735	-3.08538035663834	-3.14589075381930
F	-2.27556320982574	-1.11498451166957	-2.49689428050075
C	-3.60660652453499	-4.42133644703288	-2.91973757532300
C	-3.08556419496665	-5.05434634320329	-1.80497384491899
F	-3.82503834222336	-2.47596777066431	-4.21559056173708
F	-4.37439962315894	-5.09488431419434	-3.76933834588606
F	-1.84018510408548	-4.96347244467648	0.16053194903028
F	-3.35464565979728	-6.33888774123049	-1.58922782539090
C	-2.60138618267721	-1.96108865585421	2.61703843103917
C	-1.81500035938216	-2.12243901360222	3.79817915271581
C	-3.84570221687735	-2.50976515722347	2.79102286167999
S	-4.05296949797671	-3.19843284666380	4.33838624317997
C	-2.46723592899152	-2.76753193849568	4.80563734172675
H	-4.64846998579009	-2.54477897112151	2.07158460784233
H	-0.79843309892589	-1.76412735489015	3.88158656103850
H	-2.10035182853655	-3.01265416324059	5.79028384450214

[TS-e-FLP$^{C2\text{-}pos.}$]‡

C	-5.61278912735468	3.05771242677968	-0.50227717442957
C	-6.44029206092665	1.95889016228254	-0.65313158830802
C	-4.41695062089580	2.95057461096244	0.20063876813657
F	-5.96439686442597	4.22856667124409	-1.02452580481608
C	-6.08079187548566	0.73890943186656	-0.09189607267667
F	-7.57515162713162	2.06729142314534	-1.33613576139376
C	-4.89225806109601	0.63568696061345	0.59664980711483
C	-4.04415307757365	1.73566253183464	0.74370275302803
N	-2.93876459521881	1.39492013031291	1.51484051541579
F	-3.66002164539311	4.04146262679440	0.33787497249311
F	-6.88007172495264	-0.31736212815878	-0.22600232607194
O	-4.45963867573993	-0.47742541996220	1.19818453218704
C	-1.77577603353021	2.18872322693991	1.48437361030824
C	-1.39535542190335	2.97389368197253	2.56358622591739
C	-0.20853618427002	3.68416290811177	2.56614087165562
F	-2.16930948566426	3.03732009064011	3.63876319115224
C	0.62692394591241	3.62764514877578	1.46287129959229
F	0.13295204528786	4.41610604780288	3.61692991521178
C	0.26539043483657	2.86598330614984	0.36449314847057
F	1.76564711418557	4.30033861071206	1.45734699671984
C	-0.92320021519639	2.15670403681105	0.38567804518576
F	1.06118260031182	2.81368686267796	-0.69236047546183
F	-1.24157882238594	1.41900065088851	-0.66778966600971
Si	-2.90894531252161	-0.32986465407867	1.98596098153393
O	-1.46667619875705	-0.03983906357241	2.92578088204465
N	-1.98636574064261	-1.45376617482782	0.95644360624240
C	-0.41895774674122	-0.74845208975670	2.49892635635135
C	-0.66058806945452	-1.55545256590460	1.37600970362108
C	-2.54058617159283	-2.35763126204207	0.04363453582003
C	0.83843075058142	-0.68469251879423	3.06569116361680
F	1.06029449964078	0.07527373676946	4.13711016745760
C	1.88551025336890	-1.40524706866781	2.50415511578444
C	0.39407097156653	-2.25339037081624	0.81483616678655
C	1.66198573475602	-2.18106895735107	1.38162447064899
F	0.23560111103714	-2.99566227146178	-0.28285221818080
F	3.09973028731486	-1.33999567679862	3.03925595020603
F	2.66629073696708	-2.85606296569976	0.83284004267226
C	-3.14446233275149	-1.92319437475809	-1.13272285533212
C	-2.54806285104421	-3.72924952397277	0.28526108522634
C	-3.73934919209893	-2.80761549257995	-2.01649747741101
F	-3.15178421243768	-0.63578287514874	-1.43661303255064
C	-3.72315841970877	-4.16674089166542	-1.75122351385464
C	-3.12198695038636	-4.62900126484330	-0.59303255710221
F	-4.30747584813380	-2.36031391982012	-3.12516196545504
F	-4.27298097077205	-5.01934474890495	-2.60044650550987
F	-1.98885821141022	-4.20333309954739	1.39386144620494
F	-3.11108590766960	-5.92788819457127	-0.32248734228663
C	-3.67920783610158	-1.39958876946651	3.49637481184248
N	-5.33570984617635	0.05345459413696	5.24339407923033
C	-6.17853834531283	1.13385938861427	4.59221884541041
C	-4.53425990451432	0.50551210106633	6.45003552696614
C	-5.41710007189526	1.29391952794328	7.42702317346607
C	-3.32056152352850	1.32931561133105	6.01827603720263
C	-3.99256460195010	-0.69797878133743	7.22698950391266
C	-6.22055712561591	2.40692630171578	6.78565221690477
H	-4.76942679492642	1.68467138300954	8.21614816212561
H	-6.10596092541351	0.59748199057580	7.91671210795574
C	-7.03836507038236	1.85064358925346	5.63653283448636
C	-7.09959443235782	0.51412095132033	3.54136628856867
C	-5.30151374440699	2.14557116253019	3.85852838918905
H	-7.78907933386887	1.15575096583547	6.02785899963278
H	-7.59118432178536	2.64503601638683	5.12881422217982
H	-5.56163062468907	3.20598159153783	6.43752970685704
H	-6.87873951289810	2.86308098098662	7.52837285815471
C	-6.13687614430697	-1.12787585917383	5.56436002304842
H	-6.67229126950958	-1.46482286018216	4.68481928063529
H	-6.86357979046911	-0.94856290006509	6.36219094256119
H	-5.48364253191323	-1.94036585927126	5.86764713584989
H	-4.77792161122645	-1.27618950352499	7.71145942513088
H	-3.34102761706497	-0.31970326255996	8.01453621536553
H	-3.40120025148577	-1.36643312534172	6.60445254248124
H	-3.56041634043148	2.35769429617783	5.77280574372331
H	-2.81415531412407	0.89196145175832	5.15809256228504
H	-2.60542743868712	1.35830136446065	6.84053044757750
H	-5.91167142656085	2.68392668621195	3.13360640865979
H	-4.49565254059553	1.66301678189595	3.31428929140886
H	-4.85328475726094	2.88871828529341	4.50884597537417
H	-7.90673372051484	-0.07397303877579	3.97632281148694

H	-6.55213848350666	-0.10503545779046	2.82884464982545
H	-7.56386615856238	1.32326208866092	2.97931256524521
H	-4.37228087366538	-0.57926630192340	4.18425806785575
S	-4.78608172567910	-2.62333036103909	2.87310518449322
C	-2.75555702546860	-2.08407685301386	4.32772497383124
C	-2.96056820257221	-3.44698775483797	4.45616046163192
C	-4.04695843183570	-3.87061961050307	3.71101809581545
H	-1.94433856651468	-1.55161463279697	4.80466960527527
H	-2.33868900207838	-4.11164591365728	5.03889474506505
H	-4.40529050191786	-4.88567420923704	3.61379535764543

[TS-e-FLP$^{C3\text{-}pos}$]‡

C	-5.58388800482640	3.11773948124423	-0.44978931624252
C	-6.42699323396915	2.03296339854875	-0.61623583481037
C	-4.38916850109347	2.98278714676754	0.24961551493047
F	-5.91987956736804	4.30091547628860	-0.95379945598570
C	-6.08329130881951	0.79991087783651	-0.07496689866733
F	-7.56198210741878	2.16893311410121	-1.29317866093608
C	-4.89516900199904	0.66847942885595	0.60874344155062
C	-4.03092863610139	1.75305269902348	0.76929321419344
N	-2.93026329348544	1.38442388618750	1.53361528119141
F	-3.62012325251777	4.06188718282283	0.40890243984466
F	-6.89813724604048	-0.24407300507125	-0.22034491393878
O	-4.48597949203637	-0.45873054921328	1.20119119071088
C	-1.75079102774509	2.15387388256393	1.49823321919804
C	-1.34514813605480	2.92800249827767	2.57626863977409
C	-0.14508760813898	3.61560059079455	2.56886434171970
F	-2.10725084039814	3.00547309682907	3.65898591014028
C	0.67962712462394	3.54494497657999	1.45816413951309
F	0.21723931595818	4.34102285380876	3.61683413817703
C	0.29346237430263	2.79322859928847	0.36100627876612
F	1.83147159226988	4.19437583217506	1.44471119202228
C	-0.90866341715967	2.10758252579092	0.39171839816682
F	1.07824631869301	2.72762619277215	-0.70323963485132
F	-1.24961693778270	1.37577466497832	-0.65948893832132
Si	-2.92738024569066	-0.34916737161936	1.97505799194627
O	-1.47381705279649	-0.10249501159087	2.91086839607765
N	-2.02565339859687	-1.45299295770075	0.90897818416178
C	-0.41123040440053	-0.72253110499601	2.38943793855023
C	-0.67569778714824	-1.50424968899709	1.25587294873779
C	-2.58861618713721	-2.39441251641957	0.04182178759828
C	0.87422132718622	-0.60029765934765	2.87727051532235
F	1.12447334703909	0.14693788815270	3.95139964309509
C	1.91997268620123	-1.25450647320859	2.23600118076565
C	0.37403165934312	-2.13853917812883	0.61720491978413
C	1.66802109949834	-2.02059384023941	1.11252118874591
F	0.18177541710325	-2.86672307832823	-0.48459762315839
F	3.15919217703954	-1.13712646162569	2.70021438744074
F	2.66613834836587	-2.64322751562503	0.49444271032127
C	-3.25562732430501	-2.01497481588924	-1.11975726595160
C	-2.51840811545354	-3.75877844329892	0.31303747105092
C	-3.84318273365668	-2.94797784662856	-1.95816909690221
F	-3.32460939574763	-0.73770268729274	-1.45673680164346
C	-3.75649951936468	-4.29779005010888	-1.65944912461760
C	-3.08546537174598	-4.70538509323017	-0.51888787488107
F	-4.46966100550534	-2.55807913663954	-3.05751121673589
F	-4.30555245179512	-5.19525393229456	-2.46139081503557
F	-1.88072739484555	-4.17547742249950	1.40213855527446
F	-2.99873351785198	-5.99561943147954	-0.22549360832996
C	-3.68714782240772	-1.45639688285050	3.49466439656220
C	-2.70299468944225	-2.14039205651212	4.31745102254453
C	-4.59851890626501	-2.41915554913510	3.01731798794848
S	-4.26644789420567	-3.98080347545238	3.52223584204416
C	-2.88988890364310	-3.47235686581674	4.42001873032246
H	-5.42946258718093	-2.23113791273987	2.35551067493021
H	-1.87786488359539	-1.62225094242787	4.78298785181922
H	-2.28872905115195	-4.19691722423901	4.94697349349521
N	-5.28626588692999	0.05885828922229	5.22389721789364
C	-6.12367948967150	1.15816955532078	4.59740852185203
C	-4.50388091994017	0.46952749295122	6.45605698066143
C	-5.40101452486263	1.22412826033190	7.44606889370290
C	-3.28566494308828	1.30323280618359	6.06234177936360
C	-3.96764028985653	-0.75535885237691	7.20082716729849
C	-6.19367803932554	2.35937156367937	6.83154432960546
H	-4.76713279879005	1.58563442767298	8.25986778365094
H	-6.09823317845969	0.51054485725008	7.89841565578854
C	-6.99626746535688	1.84145230915345	5.65437206026802
C	-7.03729743739901	0.56746374701995	3.52337830339775
C	-5.24407668263165	2.19745982052793	3.90335888953281
H	-7.75187620376521	1.13480988932196	6.01404962763672
H	-7.54215996556555	2.65204346569894	5.16501011254044
H	-5.52803986297435	3.16742366658938	6.51893184189766
H	-6.86173418293417	2.79214025646044	7.57941218120858
C	-6.08254154047916	-1.13807013185072	5.47346422159671
H	-6.53923187966264	-1.47696298380940	4.54946192482119
H	-6.87854472345178	-0.98233532226899	6.20783883618129
H	-5.44206744779842	-1.94151458722677	5.82216529407961
H	-4.75565495837297	-1.34090209251879	7.67299501470639
H	-3.31221367800656	-0.40081353860611	7.99620016832770
H	-3.38215820736293	-1.41026105019739	6.55874323864804
H	-3.52768520349998	2.31526830394853	5.76023487017482
H	-2.72813798273378	0.83794301807276	5.24910479946775
H	-2.61842452568483	1.37593607433999	6.92151177932366
H	-5.83545079995801	2.71818169269005	3.15049334793135
H	-4.39526543564298	1.74488138903760	3.39917111051733
H	-4.85453424374709	2.95482347468552	4.57645577969219
H	-7.83937640630190	-0.04254959188005	3.93720842850249
H	-6.48066233217124	-0.02081105845797	2.79286482279098
H	-7.50646521802240	1.39047047089990	2.98566805851738
H	-4.30775807628692	-0.56540573490686	4.13590888099282

phenylacetylene / PhCCH

C	-5.01543329686789	1.98679113905021	0.00001738870749
C	-5.05864524750413	0.60376272523617	0.00008570767385
C	-3.79541231196844	2.64820227414197	-0.00009680769468
H	-5.93951443221028	2.55165355109034	0.00005433948108
C	-2.61460241561303	1.91900737462923	-0.00014263649179
C	-2.64918984099903	0.53575917641768	-0.00007426560082
C	-3.87389943515256	-0.13711266326394	0.00003479520204
H	-6.00683310891640	0.08177157763496	0.00017574188174
C	-3.91265112299722	-1.55961363118764	0.00007894113145
H	-1.73188154042097	-0.03871699467969	-0.00010894524382
H	-3.76485725989803	3.73077969341138	-0.00015046004155
H	-1.66031377440323	2.43119639270427	-0.00023162588998
C	-3.94101848036077	-2.76176162642952	-0.00009978984485
H	-3.96930773268797	-3.82481898875542	-0.00020238327017

[2d]$^{-}$ / [1-CCPh]$^{-}$

C	-5.17649485435484	2.67409651134590	-0.98009370054807
C	-5.90501461591574	1.50329444281205	-1.03052039055900
C	-3.88918035170225	2.68223244024344	-0.45089326987979
F	-5.70704804857783	3.80995851659117	-1.44188701671439
C	-5.35243484564128	0.32172247493949	-0.54841707075131
F	-7.13930491304114	1.50544017269831	-1.53984052827563
C	-4.07774861022982	0.32591798871063	-0.01986918312163
C	-3.32990249202567	1.51488886051999	0.03336909364204
N	-2.07475601547171	1.26284785210433	0.56429172006473
F	-3.22610479565172	3.84801002399698	-0.43715841035811
F	-6.06258872902902	-0.80650781691390	-0.60849732868848
O	-3.44963423636428	-0.74204011460752	0.44071788349744
C	-1.14392296217499	2.29110849466946	0.74770453327206
C	-1.24386813178552	3.17548698552536	1.81499032640577
C	-0.29753767621389	4.15970746557813	2.03712895254046
F	-2.26762960104597	3.08040062815734	2.65231237604558
C	0.78557229400757	4.27248130493197	1.18328766120641
F	-0.41701179842503	4.99153787221980	3.06758745086154
C	0.91239497417582	3.40279924644042	0.11411384343551
F	1.69915523286033	5.21531310275170	1.38574133760184
C	-0.04988368347656	2.43190877587059	-0.09786462212064
F	1.95625864157158	3.50964713860603	-0.70110641628271
F	0.09577708771075	1.61669921429681	-1.13224971282086
Si	-1.84483724630448	-0.44028329448888	1.09845724968469
O	-0.16661630757058	-0.07745362158494	1.47657872214443
N	-1.21752294169809	-1.90379734508561	0.24600715917101
C	0.70182030615726	-1.00746722284866	1.11533092320368
C	0.14594996718058	-2.08975289560273	0.41043304461052
C	-2.03803088350894	-2.89371691028305	-0.30264483910167
C	2.05953470880772	-0.94973682200387	1.35716493694337
F	2.59361592419717	0.08331722797471	2.01200360541814
C	2.88680454007724	-1.97366602563569	0.90881624563444
C	0.98093491914275	-3.09526036379334	-0.03908014693533
C	2.34830985264335	-3.03730885685787	0.21432474872199
F	0.51713632639198	-4.14459706968241	-0.73241216958517
F	4.19939662480302	-1.92885994439541	1.15088004497777
F	3.14348162085461	-4.01766739068804	-0.22307695388263
C	-2.69451950652215	-2.68970788245932	-1.51130641708306
C	-2.31182445384351	-4.07646286502600	0.37598557905088
C	-3.60910160048766	-3.60182450009773	-2.00588754061219
F	-2.46553820285163	-1.58866506216124	-2.21171441257337
C	-3.86637984586410	-4.76764558756149	-1.30604792171450
C	-3.21030047942923	-5.00834328244741	-0.11168588912368
F	-4.24478543208104	-3.36523911265233	-3.14795971099957
F	-4.73718480902557	-5.65235866353722	-1.78060618126414
F	-1.71376235730147	-4.32238691514171	1.53475672432368

F	-3.46361822415373	-6.12228189646875	0.56976662688818
C	-2.33742706561154	-0.80321615047277	2.83353382156816
C	-2.67496260003157	-1.12694844022780	3.95140201013934
C	-3.08094285007488	-1.53004182016518	5.25006276402592
C	-3.07672356683667	-2.88455722202796	5.60088969433899
C	-3.49965319675823	-0.58974776455729	6.19694828226245
C	-3.48184820378484	-3.28252028619302	6.86257123538078
C	-3.90458049280275	-0.99660860873279	7.45624749923032
H	-2.75457005157034	-3.61298136349464	4.86764762410236
C	-3.89816181827947	-2.34256180173095	7.79551493361363
H	-3.47330199110187	-4.33530063264975	7.11908445364825
H	-4.22847812321365	-0.25654314333057	8.17855262979261
H	-4.21618587999026	-2.65752509653306	8.78213174205519
H	-3.50359381952189	0.45855690479542	5.92695662548840

1—PhCCH

C	-5.47059739217711	2.51480933647359	-1.59564181776061
C	-5.91742665871123	1.30023533440069	-2.09040396882171
C	-4.45869990106582	2.56665467881851	-0.64523522455233
F	-6.01692365090702	3.64279294828968	-2.03052225666638
C	-5.35719770397481	0.11653166197983	-1.63103506319426
F	-6.88033277291693	1.26956657309970	-3.00224033092865
C	-4.33928033475474	0.16980574558969	-0.69872452643900
C	-3.87310867912980	1.39335354287125	-0.20078919189411
N	-2.84775290644365	1.18180876235145	0.71406234693332
F	-4.07596004658719	3.76138222718342	-0.19354877601086
F	-5.78724750327560	-1.04807293241079	-2.10261844854634
O	-3.70055263250230	-0.89615403159723	-0.21850146958024
C	-2.15994942530845	2.26250755182670	1.29207055016904
C	-2.29562635942787	2.57441596899442	2.63838869214119
C	-1.60338883617053	3.62490126291312	3.21250581841712
F	-3.10239563109343	1.85299240099937	3.40960988606139
C	-0.76817807551227	4.40613265081128	2.43065818742934
F	-1.74444294037357	3.89278034491897	4.50313827675857
C	-0.62090625570647	4.12171574877088	1.08253030751633
F	-0.11581283805085	5.42123294609508	2.97094184410711
C	-1.30542560986071	3.05227478646639	0.53210727325658
F	0.17242640736355	4.86928872189990	0.33125036944290
F	-1.14773775894139	2.78634860083513	-0.75610973791847
Si	-2.55273309015107	-0.53989028376890	1.02230128033137
O	-1.32036041928598	-0.16410866188848	2.16603686579574
N	-1.57617294945045	-1.93913381937830	0.52970927044332
C	-0.35445891325495	-1.08164626593242	2.26348300359908
C	-0.45568728846011	-2.12225907412729	1.33418840476815
C	-1.96294623597553	-2.89896688682433	-0.42091416602446
C	0.66038058846641	-1.05510936086103	3.19594282588838
F	0.74730338552311	-0.06933235469456	4.08599375854174
C	1.59826761379029	-2.08006965962562	3.21145019246046
C	0.50355859437806	-3.11807949343461	1.33262640989310
C	1.52370198250417	-3.09835033674029	2.27881867117877
F	0.48081759244407	-4.11273970446839	0.44450395414024
F	2.56281734158395	-2.08130582073469	4.12586423765426
F	2.43548233375695	-4.06483510472499	2.28356096445566
C	-1.91764187109203	-2.62354278799929	-1.78182596010694
C	-2.46774116592107	-4.13323530791234	-0.03474586513403
C	-2.37061520058274	-3.53566725913085	-2.71970275815953
F	-1.45626894808161	-1.45584991599355	-2.20306277906440
C	-2.86893918892702	-4.76062495290987	-2.30505110120010
C	-2.91157964423067	-5.06469767726092	-0.95422054129214
F	-2.33159143470770	-3.24406644631812	-4.01005727430600
F	-3.30534999598766	-5.63638030154525	-3.19434111713887
F	-2.53682295541352	-4.43596105432826	1.26042892227232
F	-3.38457959887479	-6.23443171176258	-0.54928514814456
C	-4.02842373971369	-1.04414377278640	2.40055563746153
C	-3.44269214033008	-1.53476887994829	3.37465201630771
C	-2.59539521719973	-2.00591250567745	4.37498155446043
C	-2.18706087277235	-3.35050517476781	4.38183963327109
C	-2.10303561937824	-1.10660001966122	5.33621714387531
C	-1.28537245909220	-3.77831308628385	5.33190374264372
C	-1.20452953198775	-1.55287494173986	6.28145558985403
H	-2.56804241961972	-4.02359101448693	3.62674785236303
C	-0.79430468380876	-2.88121014734498	6.27530586313165
H	-0.95189887081734	-4.80771493844685	5.33612145811247
H	-0.80434596515771	-0.86417680403798	7.01356534207366
H	-0.07554068504416	-3.22082911368028	7.01093544253808
H	-2.41073680734777	-0.07031566864493	5.29638832868376
H	-5.01903361952834	-0.82769495081825	2.04048769011297

$SiCl_4$

Cl	-2.63812601888348	1.69034430426010	1.07410212191185
Cl	-4.66217134592279	-0.79234778103269	1.89252588522590
Si	-2.73035573053119	-0.22206509139025	1.72428270720162
Cl	-1.83375420407756	-0.36362934793733	3.53044156161610
Cl	-1.78438270058498	-1.42445208389983	0.40345772404452

pmp-$SiCl_4$

Cl	-2.84850792389258	2.22663970169080	0.74606534594905
Cl	-3.38349437212566	-0.58015861360542	0.04516602768404
Si	-2.35444495240706	0.33894095367581	1.64944790378620
Cl	-3.07110597241107	1.05525223485330	3.48583530253605
Cl	-2.20130077230974	-1.63902264556726	2.52628606064658
N	-0.19623678328713	0.56553612259658	1.49851382288983
C	0.43007612125446	1.87860121039441	2.15556001715605
C	0.26008110525817	0.32555490013770	0.00906575362612
C	0.40952026228932	-0.53937837340997	2.29378876582819
H	0.17439629715293	-1.49491325088041	1.85516910467839
H	0.00816539260075	-0.53737361128312	3.29719568272686
H	1.48721499637040	-0.41695916606007	2.33177736505728
C	1.93002221039634	1.97154842682247	1.82621439847834
C	0.31922315297038	1.80787854602910	3.67955029112099
C	-0.21259939234084	3.20385114727375	1.75619302643347
C	1.77228020197407	0.53169983175811	-0.13160002043887
C	-0.44655088323169	1.22687134721870	-0.99839513337703
C	-0.02467969384546	-1.12029697983192	-0.40749172577332
C	2.25441210974769	1.87604525029893	0.35547567056069
H	1.99988409112681	0.38252489775355	-1.18915247200572
H	2.30852271443886	-0.25726856375781	0.40245366878879
H	1.78593700646336	2.68896238213427	-0.20452083732509
H	3.33138985737979	1.97103466329701	0.20176856079767
H	2.49096582537321	1.20363789485857	2.36416057677408
H	2.26581499136035	2.92222841207969	2.24371143562353
H	1.01294919351826	1.09903784636208	4.12705843835457
H	-0.69070598095328	1.58492588445742	4.01359509637929
H	0.57752069507326	2.79530196918213	4.06339983100782
H	0.72686943932678	-1.81631509286675	-0.03770443623540
H	0.01018240760099	-1.15887613303797	-1.49652094300388
H	-1.00893680025083	-1.47214071879486	-0.10910166301163
H	-0.37380411379986	2.28454743964597	-0.77663606214883
H	-1.49674815641379	0.97694871676529	-1.10970207126390
H	0.03642834953743	1.05704072387471	-1.96188598872990
H	-0.31383972616655	3.36124583631591	0.68948055925481
H	0.44072038486260	3.98691129744239	2.14425547914077
H	-1.18861128264067	3.33400551217687	2.20934316803405

[TS-N-methylpyrrole--pmp-SiCl4] ‡

Cl	-1.88845012185426	1.61839351969833	2.66776827582426
Cl	-3.80315550540202	-0.04582123809980	1.09093374712662
Si	-2.26416338937451	-0.44875654584533	2.68064840495842
Cl	-0.85088424144279	-0.59901974805661	4.37814404043176
Cl	-1.10784999305963	-1.62649397434411	1.43077186020865
C	-3.55803322462395	-1.55390152289939	3.65244708292483
C	-3.05916620397407	-2.59343014265302	4.55688182034485
C	-4.49108658572742	-2.27220722109955	2.84827101885641
N	-4.55238344522556	-3.54004926232842	3.22081639961355
C	-5.37083350189082	-4.56010829560500	2.60952967691567
H	-4.74027266153509	-5.35754938714624	2.21604674379942
H	-5.93581635155267	-4.11898058638200	1.79198166244475
H	-6.06232135429537	-4.97948073268183	3.34111054310568
C	-3.67620369534333	-3.75909119124462	4.27745688505198
H	-5.06108519518723	-1.91430192782036	2.00849063189689
H	-2.29202479900188	-2.45231507890903	5.29584615672814
H	-3.57345178202630	-4.74187789678209	4.70803248115590
N	-5.15064183352479	0.04483955312651	5.29299163240156
C	-6.11546827986731	0.97668143866715	4.57101298739310
C	-4.43897547991183	0.67592261073488	6.48098031920607
C	-5.46624045883328	1.29910879282187	7.43167822621865
C	-3.40776077174392	1.71320190097223	6.04094501800922
C	-3.64323926011737	-0.37479961942802	7.25500082533490
C	-6.40803869280408	2.27140458617893	6.74715884708297
H	-4.91801688117567	1.79392422962367	8.23726417669323
H	-6.04909892056428	0.50098817532135	7.90375122565427
C	-7.09431385207581	1.59934106952620	5.57294203538531
C	-6.92291711858431	0.20275565494647	3.52795931248786
C	-5.38496826803751	2.07113560399711	3.79190716901854
H	-7.77703887929304	0.82696497383014	5.94256889039761
H	-7.71475366930153	2.31448862253260	5.02673984724147
H	-5.85939593391351	3.15392570029623	6.40997805517624
H	-7.15473524788850	2.63214779881685	7.45826082328984
C	-5.83071821393917	-1.19126047324564	5.68393694123246
H	-6.17267734518444	-1.70949560633396	4.79274092387524
H	-6.69016520759132	-1.02456254672349	6.33631682330932
H	-5.13299015437026	-1.85316809038268	6.18194544973729

H	-4.26446849641692	-1.12344693872474	7.74435300834787
H	-3.09239246225623	0.14195606297192	8.04054402113892
H	-2.90817079570514	-0.86251635036684	6.61680529073353
H	-3.83605590524141	2.64393756086457	5.68949672564234
H	-2.74929509230884	1.32260893496745	5.26772505185888
H	-2.78367533063256	1.95537406625865	6.90179307547206
H	-6.05014349975084	2.43854329541421	3.01025098580302
H	-4.49136940880861	1.69686410783899	3.29912988472923
H	-5.11134709211555	2.92809693933651	4.39837122348802
H	-7.56610926329413	-0.56646667075712	3.95246175243168
H	-6.27138915921260	-0.22965125416369	2.76948481691280
H	-7.57315272563068	0.91517524298516	3.02045735261769
H	-4.19725324838740	-0.63458113970435	4.33816982329073

$Si(cat^{Cl})_2$

C	-10.55076226899912	0.78474120843701	0.58941316723326
C	-10.32192076373243	-0.26402232745372	-0.30551672408844
C	-9.49242808187249	1.58639506353077	1.03828296613970
Cl	-12.13054033257647	1.10013381293036	1.15412754240195
C	-8.22701633776459	1.30798477723132	0.56758562509050
Cl	-9.71821646241455	2.86754906165697	2.13871197245663
C	-7.99854764926496	0.26259246221636	-0.31997501836773
O	-7.09234276084206	1.98771513029024	0.90899787363372
C	-9.02815910453218	-0.53581941315068	-0.77126876020853
Cl	-11.62218121222198	-1.23235354609910	-0.84107427012257
Cl	-8.69533513587660	-1.80526628150983	-1.85826082257715
O	-6.68579369104490	0.12561484992972	-0.66706494856490
Si	-5.82161605332537	1.26571628184880	0.14932912380924
O	-4.86374660199015	2.23183277927610	-0.77946702878949
O	-4.63977633534676	0.69057005630793	1.14221989392336
C	-3.57798966416672	2.09807883374492	-0.33768321195948
C	-3.45309994784435	1.23392218651950	0.74401401361560
C	-2.48111383663270	2.73320364158393	-0.87961784494474
C	-1.22661745915061	2.47945986589287	-0.30804253041050
Cl	-2.68727199839297	3.78404021275667	-2.20481833397723
C	-1.10210170802665	1.61512634164667	0.78307771393870
Cl	0.15510219764143	3.24004165746373	-0.96178651697196
C	-2.22846407955967	0.98102479266969	1.32471934766495
Cl	-2.13179287633742	-0.07557414424355	2.65814174664372
Cl	0.43228216427440	1.31872269652327	1.47046502443140

pmp-$Si(cat^{Cl})_2$

C	-4.51408413527720	3.39562732711956	-0.30494924656535
C	-5.42867282123843	2.52507062486062	-0.89977548242426
C	-3.82013840647957	3.01851418418844	0.85387529411936
C	-5.66644784457383	1.25815035803815	-0.34654147611134
C	-4.96505706552679	0.89923514245819	0.78462869776242
C	-4.05233854282212	1.76341795257706	1.37883545103958
O	-3.51839049424180	1.25228403638717	2.48528162955952
O	-5.08561256863212	-0.24954820585042	1.46386739918540
Si	-4.05332981158499	-0.35547998198333	2.82308689574352
O	-2.43432518159686	-0.84011678043963	3.01587835588699
O	-4.54293340398876	-2.02471599648449	2.89424072441702
C	-2.30618607639370	-2.16049548649638	3.23886674517642
C	-3.52360148239692	-2.83267174938471	3.16875321509739
C	-1.13542209580671	-2.82390652273773	3.53737135091640
C	-1.19157473588225	-4.20732211721868	3.76471775952143
C	-3.59359335703270	-4.19231925728206	3.40297890684380
C	-2.41014303873138	-4.88347280450510	3.69808538624946
N	-4.79633011061108	0.06371774372700	4.66171529386309
C	-6.22808011309093	0.69818908970215	4.52683052575516
C	-3.82017967871752	0.88397318036623	5.62817614533113
C	-4.56504268028051	1.24783256587896	6.92005126026671
C	-3.22277262674817	2.16187311524575	5.04134872097749
C	-2.62385559661875	0.01873045852467	6.02663687098587
C	-5.88052671625709	1.96012655819635	6.70686970141533
H	-3.87492203907003	1.86516134436315	7.49736221338516
H	-4.73421265057296	0.35488324385458	7.52660918627209
C	-6.78638370286483	1.05499947733804	5.90577423184758
C	-7.19363567968500	-0.30047566185178	3.88302564588874
C	-6.24356406988697	1.94403368932433	3.64702968630089
H	-6.99114425643470	0.14494075235941	6.47557218658106
H	-7.75892847269809	1.51907033439471	5.73011791077033
H	-5.72910809533317	2.91238166202317	6.19265764013482
H	-6.33784006664364	2.19627906274099	7.66969732596276
C	-4.98368589340159	-1.25401796761878	5.34452865995866
H	-5.70984928155877	-1.85152006079224	4.81610348849920
H	-5.30921216955298	-1.10215106462258	6.36792708077960
H	-4.05098935973846	-1.80298660222474	5.35308800275494
H	-2.88707534083884	-0.80975003228832	6.68049775917305
H	-1.94418138282039	0.66064515797540	6.58744860238919
H	-2.07450442716712	-0.35124803743476	5.16527157525113
H	-3.94427734882274	2.87739125066568	4.66737073116642
H	-2.51033138171222	1.96032376976905	4.25092196362148
H	-2.68859961831884	2.64600393649098	5.86016532152449
H	-7.22599839034101	2.40391908594940	3.75915133075460
H	-6.13717772330952	1.70300151390995	2.59427423572366
H	-5.50397093955572	2.69087192115752	3.90292510282483
H	-7.52601291498932	-1.07288421477329	4.57436477391668
H	-6.79458987008506	-0.77295553559780	2.98682409167748
H	-8.07912579535701	0.25918419571759	3.57988089715448
Cl	0.32668960150826	-1.94251458203653	3.63029059081598
Cl	0.24617203098131	-5.05646845625517	4.13699510448329
Cl	-2.47593865836885	-6.56795107173532	3.98895553967569
Cl	-5.11547963511083	-4.97097676279161	3.34446571539656
Cl	-6.79888355605809	0.16682367295400	-1.01457384830545
Cl	-6.27822139291980	2.99622451121939	-2.30789566439854
Cl	-4.23704341225932	4.94389480850910	-0.97864053167339
Cl	-2.72085552248309	4.06635322441868	1.64214332467965

[TS-N-methylpyrrole--pmp-$Si(cat^{Cl})_2$]‡

C	-6.09929100377534	2.78945006951128	-0.39727077856197
C	-6.72144716985352	1.59913508395777	-0.76936303127955
C	-4.91596751141841	2.76429267683934	0.35822650403730
C	-6.16867098714737	0.36440462679652	-0.40207460127893
C	-4.99381306343281	0.34898122134065	0.32475503325935
C	-4.38719826111849	1.54265987105189	0.71522537390518
O	-3.30797793724841	1.34305689295791	1.48136978373659
O	-4.36273347181927	-0.72113698101661	0.78285820557630
Si	-2.99082493946752	-0.30136254688611	1.82035661328170
O	-1.64532507118412	0.24172327314324	2.82146714068155
O	-1.93058151872374	-1.25902375358884	0.89984392487274
C	-0.55566824490425	-0.45965962457219	2.54497527839008
C	-0.70588768678002	-1.31330634452258	1.44682537264202
C	0.62967053921005	-0.43653204335203	3.25616868859954
C	1.68858478421337	-1.25525885195231	2.84153717563746
C	0.32601589031471	-2.13027405027495	1.03525997409664
C	1.54232825390177	-2.09010252750587	1.73554501029844
C	-3.70407307679606	-1.36193119138812	3.28616331582798
C	-2.70776967293205	-2.12126279960002	4.03948490120310
C	-4.62228071146957	-2.36595681627756	2.87730465219766
N	-4.24006463592978	-3.55542770307674	3.32298413339135
C	-4.90704719159072	-4.81054377073861	3.06438976633130
H	-4.23773499441286	-5.48507976569838	2.53063920790998
H	-5.78537752440282	-4.62528785174628	2.45081870416311
H	-5.21353278202013	-5.27637571229838	4.00131699461501
C	-3.06138261659867	-3.42528869045235	4.04597201538861
H	-5.48830216337581	-2.26718813114229	2.24256519199008
H	-1.82722210595078	-1.70683065693830	4.50213768402030
H	-2.58641000356919	-4.29241832951063	4.47550661679782
N	-5.10622075515694	0.12449016794655	5.15039443576880
C	-5.90798063615679	1.28992249771857	4.59549850997099
C	-4.27088339581402	0.45511294110202	6.37520116013280
C	-5.13000058192043	1.17024806324026	7.42683988684530
C	-3.04095679299440	1.27937334808383	5.99047383155113
C	-3.74187041517261	-0.82115340133509	7.03351767146118
C	-5.94167533434041	2.33871645203789	6.90100555515821
H	-4.46566783942942	1.49314459434658	8.23257243235308
H	-5.81286105934715	0.43994353698280	7.87445534285976
C	-6.76643278364722	1.90751165994242	5.70208110846058
C	-6.81741607224966	0.79500964582770	3.46966305820973
C	-5.00427501863443	2.36641208429708	3.99305379124241
H	-7.52689150341134	1.18705434273102	6.02092986263099
H	-7.30631816014843	2.75599952864779	5.27447274168445
H	-5.28616713642489	3.17101623732318	6.63562145122387
H	-6.59711790787200	2.71375679494330	7.69018205786403
C	-5.95380957528899	-1.04108756842678	5.40040294225839
H	-6.53111754703053	-1.27362950695904	4.51253043787555
H	-6.64445465927045	-0.90127735563299	6.23484913995044
H	-5.32423481176014	-1.90179320710415	5.60819857657758
H	-4.52915650694301	-1.42947812336280	7.47728872037841
H	-3.07432508742630	-0.52329869198054	7.84178242119397
H	-3.16938553894487	-1.43563562985292	6.34209437504931
H	-3.25914294669755	2.32540221347188	5.80722015055089
H	-2.54516626351391	0.87838317937023	5.10608950421261
H	-2.32703976006800	1.24185156634621	6.81367723924520
H	-5.58915978320377	2.95815737917658	3.29004142854140
H	-4.16148747238994	1.95428842031301	3.44674918494303
H	-4.61630932052785	3.06086288940140	4.73072806856981
H	-7.65609823316153	0.19947828019075	3.82886527733064
H	-6.26648194574076	0.21989632817228	2.72434424957030
H	-7.23652884758679	1.65960722296097	2.95682772015585
H	-4.28615695173076	-0.48670893325090	4.07912589730662
Cl	0.74324755623156	0.57225139802027	4.63769537710479

Cl	3.16148774891039	-1.22846521040497	3.71558238835144
Cl	2.84217479628593	-3.08356673709739	1.22751418271361
Cl	0.08465301735695	-3.17513502248397	-0.29822885682264
Cl	-6.92281622403290	-1.12507184080785	-0.79212125276954
Cl	-8.17294284712952	1.63165947693540	-1.67794248396757
Cl	-6.77636203723204	4.29576377273398	-0.85011770698532
Cl	-4.12965642810267	4.19903163337593	0.85868126951671

[Si(cat^{Cl})$_2$····pmp]^{vdw} (van-der-Waals adduct)

C	-6.51794305537849	1.89749238983405	-0.06703695251790
C	-7.03964820853397	0.61332519110078	0.10599859834096
C	-5.19074199476584	2.18146778819391	0.28167791761187
C	-6.24498482698936	-0.41572688630644	0.62956089749044
C	-4.94237581589641	-0.12007711176825	0.96979139050953
C	-4.42384898914240	1.15861631673178	0.79685626540691
O	-3.11517273179509	1.26754925639596	1.16394023125738
O	-4.03831266949678	-1.00970726064939	1.47078108915224
Si	-2.59518552521459	-0.22984074780814	1.61134737644570
O	-1.79158469851450	-0.34921104197703	3.04294524206485
O	-1.39748226096922	-0.85422889055748	0.66046955619005
C	-0.55834173659779	-0.88461216781803	2.79944696063948
C	-0.33900729711426	-1.16804286515715	1.45642602522429
C	0.40545953509618	-1.13362559898446	3.75287726297904
C	1.62143391113722	-1.68694470008882	3.32814589325139
C	0.85109702400148	-1.71197890569224	1.02242990096488
C	1.84132944966635	-1.97340538679946	1.97873757119611
N	-5.16246672712361	0.67515321734591	4.65816925169390
C	-5.93923875324586	1.95226190718074	4.61790398288978
C	-4.29250120643417	0.50364002491955	5.86159776108852
C	-5.05989716275666	0.78427130225532	7.16181468968857
C	-3.05369675905570	1.40263887165841	5.78705463744932
C	-3.75961001907679	-0.92779851908913	5.93562764304599
C	-5.75273034892012	2.13329339169529	7.15336013158418
H	-4.36628787991743	0.70646371661431	8.00395960855332
H	-5.81071450479326	-0.00076642949120	7.30655594987343
C	-6.66265840804057	2.22916208923453	5.94415851365330
C	-7.00602696372918	1.89999924853233	3.52616430656464
C	-5.02797548043206	3.13009053970119	4.24159234879649
H	-7.47365908360032	1.50041274692474	6.05509877982753
H	-7.13737859884761	3.21312046325750	5.88815835199769
H	-5.01556054175677	2.94091181214719	7.14171396022095
H	-6.33180226404441	2.26592603507064	8.07064712767639
C	-5.98965847686016	-0.49379493524704	4.41016383245734
H	-6.54015167025608	-0.37297057048077	3.48344905247434
H	-6.72123542445313	-0.72213501582326	5.20227980565360
H	-5.36464932053383	-1.37116284285269	4.27333299581960
H	-4.53899247063091	-1.65620397425100	6.15713352550020
H	-3.02631767191025	-0.98393524608114	6.74066322244872
H	-3.25729359109536	-1.21338500280902	5.01081238888518
H	-3.26099561893812	2.44903833418940	5.98410686700142
H	-2.58230182252039	1.32258944693414	4.80931717744708
H	-2.33170505283919	1.07615218521750	6.53724509307148
H	-5.63026261658865	3.94458252957210	3.83658122896872
H	-4.31283317957943	2.82178203706832	3.47885766238622
H	-4.47182637020183	3.53795290214576	5.08098724261533
H	-7.80573520364528	1.19289457700857	3.74324282292089
H	-6.56641032571962	1.64914592865448	2.56201916747206
H	-7.46110798454191	2.88669104491434	3.43646655408306
Cl	0.09656700366242	-0.76575828230118	5.38741734081040
Cl	2.83852443969071	-2.00553617471050	4.48253958728337
Cl	3.32702835636263	-2.64715318817104	1.47574361499178
Cl	1.07003057695840	-2.03925657301166	-0.63532616852733
Cl	-6.83577450493534	-1.99746343919401	0.85949182043136
Cl	-8.66616867064566	0.28720301852104	-0.29726482297504
Cl	-7.50389983274452	3.14805886255083	-0.68173248784381
Cl	-4.51298597575145	3.73460458154976	0.10895020581183

Si(cat^{Cl})$_2$····C$_4$H$_4$NCH$_3$

C	-4.32125661722559	3.60529021529790	0.68552638718794
C	-5.31767449374937	2.85039536531268	0.06545803336140
C	-3.42501503612231	3.00146433600083	1.57759424637032
C	-5.43969709504295	1.47760713598803	0.33174015140194
C	-4.54708963727090	0.89931629142587	1.20892222921060
C	-3.54578180286774	1.64864346885891	1.81939328087331
O	-2.78931868253082	0.92304484301924	2.64314773044024
O	-4.54120423581141	-0.38594302515414	1.60259647405339
Si	-3.41155779930700	-0.68235242054040	2.82935041690909
O	-1.83505608424907	-1.29576316774236	2.94100721357499
O	-4.06773059011961	-2.27577202257099	3.01418283094048
C	-1.83796399480731	-2.57721951442591	3.35039522970306
C	-3.11778593579938	-3.12850678152860	3.39958330828022
C	-0.72566476679291	-3.30624649250025	3.71542373985125
C	-0.90432791981170	-4.63245675800088	4.13160522254775
C	-3.30665130100183	-4.43149507205190	3.82289589030419
C	-2.18416336601612	-5.18763130074527	4.18633053916410
N	-3.17492097779997	0.74987148429630	5.34200594136937
Cl	0.81478599779834	-2.56713597363723	3.65824732351327
Cl	0.45984122771182	-5.56059951716813	4.58208142090330
Cl	-2.39653400794282	-6.80127851226006	4.71168342969782
Cl	-4.89253018429280	-5.06425298243255	3.89029259179004
Cl	-6.65989189677628	0.51723499895744	-0.38004823881644
Cl	-6.41019709653142	3.59333847842537	-1.02148872444329
Cl	-4.18633655651132	5.28147984561515	0.36934744999540
Cl	-2.20877595953126	3.88654384450686	2.39758805442653
C	-1.76228433342687	0.67399151689815	5.64074699986894
C	-3.91857047469311	-0.32404703099213	4.84014154014934
C	-3.89548609357932	1.85922185883423	5.25660121377744
C	-5.18164162740876	1.55906702412929	4.79525144224711
C	-5.22206707874566	0.19705446915873	4.58458229038170
H	-1.19229394943852	0.62840501907455	4.71244011998691
H	-1.56316689741522	-0.21946815525421	6.23055526729785
H	-1.47125394290204	1.55308135259356	6.21067276106017
H	-3.46021033308273	2.82193184275414	5.47796793673260
H	-5.96941579979586	2.27332298984586	4.62212196373241
H	-3.71835796949031	-1.30293186736187	5.26329979927956
H	-6.05295268761962	-0.39525578662619	4.23306649287548

[Si(cat^{Cl})$_2$— C$_4$H$_4$NCH$_3$$^{C3\text{-}pos.}$]$^-$

C	-6.12579142851423	2.43314169853371	0.08604289216122
C	-6.48401401750161	1.34904830727022	-0.70650337417272
C	-5.01441915472850	2.34586171465191	0.94182824920963
C	-5.73585026521078	0.16284658849426	-0.66682829236200
C	-4.63685284250027	0.07947368850928	0.17098660861244
C	-4.29074414004817	1.17257830919278	0.98467499058533
O	-3.23240361748523	0.93224740491070	1.75225461823854
O	-3.83978056346337	-0.95092258999078	0.31747363024813
Si	-2.68152787698312	-0.70125869882597	1.66973178060326
O	-1.39783690166019	-0.25561048406799	2.83589144885670
O	-1.43993795515277	-1.22715625334079	0.59495657579297
C	-0.20707422229937	-0.60153330180762	2.40903184796591
C	-0.21967699094126	-1.15919806801253	1.11947787329089
C	0.98948317038651	-0.46944750789249	3.09327962191696
C	2.18163134434849	-0.88616442550374	2.48193046627426
C	0.94874305519524	-1.56595898019763	0.51105603792258
C	2.16435842146027	-1.42615109898147	1.20115182742900
C	-3.48888715727630	-1.93402271338975	2.77852830646337
C	-3.14430692883188	-2.29901302724350	4.11427127852541
C	-4.59888235184971	-2.69158852282564	2.46243406339540
N	-4.92891326660479	-3.47415989170532	3.52390014866652
C	-5.99509673902097	-4.43482214297469	3.55196062258179
H	-5.61272204778271	-5.45890696954604	3.52143890618712
H	-6.63580321421637	-4.27814325204220	2.68566215786862
H	-6.59871473334428	-4.31328303663681	4.45367325055067
C	-4.04079799642875	-3.24141479874975	4.54217948829845
H	-5.16962298250957	-2.72697463079485	1.54826664697244
H	-2.32744336326200	-1.88753177065652	4.68519794290034
H	-4.13181169227325	-3.76468448278194	5.48119056031697
Cl	0.96863414892944	0.19705232989180	4.67529690520640
Cl	3.66765686256120	-0.72948622631618	3.33321051984111
Cl	3.62655041619682	-1.92985333916690	0.45008595838680
Cl	0.88100383085249	-2.23325657875058	-1.06874198949118
Cl	-6.15453126986967	-1.20521911482574	-1.61835339087603
Cl	-7.85647099467254	1.44764944759656	-1.73800553000992
Cl	-7.04519629524675	3.88518188919376	0.03773242711851
Cl	-4.54314023980191	3.66058052878248	1.93972492452404

[Si(cat^{Cl})$_2$— C$_4$H$_4$NCH$_3$$^{C2\text{-}pos.}$]$^-$

C	-6.34107962790680	2.89269716398294	0.52795368722545
C	-6.75619333319765	1.80575707243265	-0.23338813192901
C	-5.15503537358145	2.82287472292141	1.27762294882651
C	-5.99285684482592	0.62884378877165	-0.26193664688662
C	-4.82527880287249	0.56599026081220	0.47378764845686
C	-4.41155285346152	1.66010019773472	1.24856544798608
O	-3.27092968125008	1.43705786843576	1.88456505245029
O	-3.98889845952318	-0.44998929788032	0.53235907399055
Si	-2.72427213992348	-0.20980369202958	1.74984350285882
O	-1.22673819636407	0.37087219719272	2.48123609600852
O	-1.75270904129251	-1.24767999715792	0.73759480620020
C	-0.20456690134684	-0.40264098276079	2.17603310513276
C	-0.50116513701831	-1.33555837089819	1.17044306509123
C	1.06322036254538	-0.35238497254848	2.72531347355901
C	2.04255879993393	-1.24817319144858	2.26873441051537
C	0.45710059320643	-2.21721472077660	0.71578291107181
C	1.74458074474701	-2.17227705737613	1.27347001636139

C	-3.26157022883758	-0.94494099026177	4.51317176194539
C	-3.91014950875759	-1.96690794165523	5.23633649011901
C	-3.38249043267057	-1.21980820109386	3.16133871399274
N	-4.08748766503832	-2.39859786215722	3.06509509118710
C	-4.44558771752380	-3.07947071949704	1.84390904631659
H	-3.61142419348354	-3.06071540656544	1.14431037659942
H	-5.30218073632478	-2.60904632193509	1.35951346539816
H	-4.68844296608215	-4.11478626700745	2.08166755492976
C	-4.40580491061958	-2.85113786445528	4.30672436392660
H	-3.99606410063904	-2.05937861150331	6.30769420387356
H	-4.95001928079792	-3.77441826234482	4.43037254840506
Cl	1.39268843996817	0.80198294174614	3.95043893866622
Cl	3.61695778066743	-1.19777939566458	2.95572031216107
Cl	2.94376709954362	-3.27183175932939	0.71971833969595
Cl	0.04115093615381	-3.34322796219282	-0.51124884527402
Cl	-6.46869177891617	-0.74040691805415	-1.18273735516398
Cl	-8.21094653359720	1.88886901275985	-1.14456264297377
Cl	-7.27891471462665	4.33249820538915	0.56193632206835
Cl	-4.60861069301661	4.14416496262501	2.22513169152427
H	-2.74253290326979	-0.08965162821016	4.91667735568314