Supporting Information

for

A zwitterionic disilanylium from an unsymmetric disilene

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Content

General Experimental Information. All experiments were carried out under argon atmosphere using Schlenk techniques or inside a MBRAUN glove box. Toluene and *n*-hexane, were purified by MBRAUN solvent purification system MB SPS-800 and stored over activated 4 Å molecular sieves prior to use. Benzene-d_6 was distilled over Na/benzophenone and stored over activated 4 Å molecular sieves prior to use. The precursors, [PhC(N*t*Bu)$_2$SiSi(Si(Me)$_3$)$_3$] (**1**)[1] and [PhC(N*t*Bu)$_2$SiCl] (**1′**)[2] and (SiMe$_3$)$_3$SiK·2thf,[3] were synthesized by using literature procedure. Chemical purchased from Sigma Aldrich and TCI Chemicals were used without further purification. ^{1}H, ^{13}C, ^{29}Si, and ^{77}Se NMR spectra were recorded in C_6D_6 using a Bruker Advance DPX 200 or a Bruker Advance DRX 400 or 500 spectrometers. Melting points were measured in a sealed glass tube using Stuart SMP-30 melting point apparatus.

Synthesis of [PhC(NtBu)$_2$]Si(CH$_2$SiMe$_3$)=Si(SiMe$_3$)$_2$ (2). To the 20 mL toluene solution of 1 (1.000 g, 1.97 mmol), 5 mL toluene solution of Me$_3$SiCH2Cl (0.242 g, 1.97 mmol) was added drop by drop at room temperature. The dark orange-red reaction mixture was allowed to stir for 12 h. After that all the volatiles were removed under reduced pressure, dried for 1 h and the residue was extracted with *n*-hexane (10 mL). The solution was filtered through cannula and the resulting filtrate concentrated to ~3 mL and stored at -4°C in a freezer for overnight to isolate red crystals of 2 (0.802 g, 78% yield). Mp: 84-85 °C. ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 7.46-7.44 (d, $^3J_{H-H}$ = 7.63 Hz, 1H, Ph), 7.12-7.10 (d, $^3J_{H-H}$ = 8.39 Hz, 1H, Ph), 6.98-6.95 (m, 1H, Ph), 6.91-6.87 (m, 2H, Ph), 1.19 (s, 18H, *t*Bu), 0.89 (s, 2H, CH$_2$SiMe$_3$), 0.68 (s, 18H, Si(SiMe$_3$)$_2$), 0.28 (s, 9H, CH$_2$SiMe$_3$) ppm; ^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 298 K): δ 172.0 (NCN), 134.4 (Ph), 129.6 (Ph), 129.3 (Ph), 53.9 (CMe$_3$), 32.1 (CMe$_3$), 9.1 (CH$_2$SiMe$_3$), 2.4 (CH$_2$SiMe$_3$), -1.1 {=Si(SiMe$_3$)$_2$}, -1.3 {=Si(SiMe$_3$)$_2$} ppm; ^{29}Si{^{1}H} NMR (99.3 MHz, C_6D_6, 298 K): δ 65.1 {s, LSi(CH$_2$SiMe$_3$)=*Si*(SiMe$_3$)$_2$}, -0.02 {s, LSi(CH$_2$SiMe$_3$)=Si(*Si*Me$_3$)$_2$}, -1.1 {s, LSi(CH$_2$*Si*Me$_3$)=Si(SiMe$_3$)$_2$}, -7.0 {s, L*Si*(CH$_2$*Si*Me$_3$)=Si(SiMe$_3$)$_2$} ppm. Elemental Analysis: calcd. C, 57.62; H, 10.06; N, 5.38; found C, 57.93; H, 10.31; N, 5.21.

Synthesis of [PhC(N*t*Bu)$_2$]Si(CH$_2$SiMe$_3$)Cl$_2$ (3). To the 20 mL toluene solution of [PhC(N*t*Bu)$_2$SiCl] (**1′**) (0.500 g, 1.69 mmol), toluene solution (5 mL) of Me$_3$SiCH$_2$Cl (0.210 g, 1.69 mmol) was added at room temperature. The resultant reaction mixture was heated at 60 °C for 12 h with vigorous stirring. Upon completion, the solution was filtered through cannula and the resulting filtrate was concentrated to ~2 mL to get colorless crystal of **3**, suitable for single crystal X-ray analysis (0.642 g, 90% yield). Mp: 228-229 °C. ^{1}H NMR (500 MHz, C_6D_6, 298 K): δ 6.93-6.91 (m, 3H, Ph), 6.85-6.84 (m, 2H, Ph), 1.20 (s, 18H, *t*Bu), 1.08 (s, 2H, CH$_2$SiMe$_3$), 0.43 (s, 9H, CH$_2$SiMe$_3$) ppm; ^{13}C{^{1}H} NMR (125.7 MHz, C_6D_6, 298 K): δ 168.9 (NCN), 127.9 (Ph), 126.9 (Ph), 125.7 (Ph), 53.8 (CMe$_3$), 30.4 (CMe$_3$), 15.3 (CH$_2$SiMe$_3$), 0.04 (CH$_2$SiMe$_3$) ppm; ^{29}Si{^{1}H} NMR (99.3 MHz, C_6D_6, 298 K): δ 0.05

{LSi(CH_2SiMe_3)Cl_2}, -74.3 {L*Si*(CH_2SiMe_3)Cl_2} ppm. Elemental Analysis: calcd. C, 54.65; H, 8.21; N, 6.71; found C, 54.52; H, 8.43; N, 6.69.

Synthesis of [PhC(N*t*Bu)$_2$]Si(=S)CH_2SiMe_3 (4). 8 mL of toluene was added to the mixture of **2** (0.200 g, 0.38 mmol) and S (13 mg, 0.38 mmol) at -78 °C. The reaction mixture was allowed to reach room temperature slowly and stirred further for 2-3 h. After that, the yellow colored solution was reduced to half, the filtrate was separated using a cannula and then kept for crystallization at -4 °C to get pale yellow crystals of **4** (0.070 g, 48% yield). Mp: 139-140 °C. 1H NMR (400 MHz, C_6D_6, 298 K): δ 6.98-6.95 (m, 2H, Ph), 6.92-6.87 (m, 2H, Ph), 6.82-6.81 (m, 1H, Ph), 1.13 (s, 18H, *t*Bu), 0.68 (s, 2H, CH_2SiMe_3), 0.50 (s, 9H, CH_2SiMe_3) ppm; $^{13}C\{^1H\}$ NMR (100.6 MHz, C_6D_6, 298 K): δ 173.5 (NCN), 131.0 (Ph), 130.4 (Ph), 129.3 (Ph), 125.7 (Ph), 55.0 (CMe_3), 31.4 (CMe_3), 9.4 (CH_2SiMe_3), 1.9 (CH_2SiMe_3) ppm; $^{29}Si\{^1H\}$ NMR (99.3 MHz, C_6D_6, 298 K): δ 19.4 {s, L*Si*(CH_2SiMe_3)=S}, 0.02 {s, LSi(CH_2SiMe_3)=S}ppm. Elemental Analysis: calcd. C, 60.26; H, 9.05; N, 7.40; found C, 60.10; H, 8.85; N, 7.98.

Synthesis of [PhC(N*t*Bu)$_2$]Si(=Se)CH_2SiMe_3 (5). 8 mL of toluene was added to the mixture of **2** (0.200 g, 0.38 mmol) and Se (13 mg, 0.38 mmol) at -78 °C. The reaction mixture was allowed to reach room temperature slowly and stirred further for 5-6 h. After that, the pale yellow colored solution was reduced to half, the filtrate was separated using a cannula, and kept for crystallization at -4 °C to get colorless crystals of **5** (0.080 g, 49% yield). Mp: 198-199 °C. ^1H NMR (400 MHz, C_6D_6, 298 K): δ 6.96-6.92 (m, 2H, Ph), 6.89-6.84 (m, 2H, Ph), 6.82-6.81 (m, 1H, Ph), 1.15 (s, 18H, tBu), 0.79 (s, 2H, CH_2SiMe_3), 0.49 (s, 9H, CH_2SiMe_3) ppm; $^{13}C\{^1H\}$ NMR (100.6 MHz, C_6D_6, 298 K): δ 171.3 (NCN), 129.2 (Ph), 128.4 (Ph), 126.4 (Ph), 53.3 (CMe_3), 29.5 (CMe_3), 9.5 (CH_2SiMe_3), -0.09 (CH_2SiMe_3) ppm; $^{29}Si\{^1H\}$ NMR (99.3 MHz, C_6D_6, 298 K): δ 20.3 {s, L*Si*(CH_2SiMe_3)=Se}, 0.4 {s, LSi(CH_2SiMe_3)=Se} ppm; $^{77}Se\{^1H\}$ NMR (76.3 MHz, C_6D_6, 298 K): δ - 413.7 ppm. Elemental Analysis: calcd. C, 53.62; H, 8.05; N, 6.58; found C, 53.45; H, 8.01; N, 6.86.

Synthesis of [PhC(N*t*Bu)$_2$]Si(CH_2SiMe_3)-SiTe($SiMe_3$)$_2$ (6). 8 mL of toluene was added to the mixture of **2** (0.200 g, 0.38 mmol) and Te (13 mg, 0.38 mmol) at -78 °C. The reaction mixture was allowed to reach room temperature slowly and stirred further for 6 h. After that, the orange-red colored solution was reduced to half, the filtrate was separated using a cannula and then kept for crystallization at -4 °C to get red crystals of **6** (0.088 g, 35% yield). Mp: 79-80 °C. ^1H NMR (400 MHz, C_6D_6, 298 K): δ 7.69 (d, J = 7.7 Hz, 1H), 7.12-7.10 (m, 1H, Ph), 7.01-6.97 (m, 1H, Ph), 6.92-6.87 (m, 2H, Ph), 1.39 (s, 2H, CH_2SiMe_3), 1.20 (s, 18H, *t*Bu), 0.67 (s, 18H, Si($SiMe_3$)$_2$), 0.15 (s, 9H, CH_2SiMe_3) ppm; $^{13}C\{^1H\}$ NMR (100.6 MHz, $CDCl_3$, 298 K): δ 172.2 (NCN), 129.4 (Ph), 128.4 (Ph), 126.8 (d, Ph), 126.7 (Ph), 54.0 (CMe_3), 30.3 (CMe_3), 29.6 (CH_2SiMe_3), 0.09 {Si($SiMe_3$)$_2$, - 0.09 (CH_2SiMe_3) ppm; $^{29}Si\{^1H\}$ NMR (99.3 MHz, C_6D_6, 298 K): δ 21.2 {s, L*Si*(CH_2SiMe_3)=SiTe($SiMe_3$)$_2$}, 1.5 {s, LSi(CH_2SiMe_3)=SiTe($SiMe_3$)$_2$}, 0.35 {s, LSi(CH_2SiMe_3)=SiTe(*Si*Me_3)$_2$}, -20.4 {s,

LSi(CH_2SiMe_3)=*Si*Te($SiMe_3$)$_2$} ppm; ^{125}Te{^{1}H} NMR (126.3 MHz, C_6D_6, 298 K): δ -396.8 ppm. Elemental Analysis: calcd. C, 46.29; H, 8.08; N, 4.32; found C, 47.12; H, 8.94; N, 5.09. Due to the air and moisture sensitivity of the crystals, the obtained values deviate from the calculated ones.

Synthesis of [PhC(N*t*Bu)$_2$]Si(H)(CH_2SiMe_3)-Si(TeBcat)($SiMe_3$)$_2$ (7). To the 0.6 mL C_6D_6 solution of **6** (0.060 g, 0.09 mmol) taken in a NMR tube, HBcat (0.012 g, 0.09 mmol) was added drop by drop at room temperature. The colour of the reaction mixture was started changing from red to pale green over 15 min to afford compound **7**.

N.B. The formation of **7** is always accompanied by PhC(N*t*Bu)$_2$Bcat (**8**).

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 7.08-7.06(m, 2H, Ph), 6.95-6.92 (m, 2H, Ph), 6.88-6.86 (m, 3H, Ph), 6.78-6.77 (m, 2H, Ph), 3.01 (s, 1H, SiH), 1.18 (s, 18H, *t*Bu), 0.93 (s, 2H, CH_2SiMe_3), 0.41 (s, 9H, CH_2SiMe_3), 0.29 (s, 18H, Si($SiMe_3$)$_2$) ppm; ^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 298 K): δ 172.7 (NCN), 131.4 (Ph), 130.5(Ph), 128.6 (Ph), 128.4 (Ph), 128.0 (Ph), 123.0 (Ph), 112.8 (Ph), 55.8 (CMe_3), 31.6 (CMe_3), 15.2 (CH_2SiMe_3), 2.0 {Si($SiMe_3$)$_2$, 1.2 (CH_2SiMe_3) ppm; ^{11}B NMR (128.3 MHz, C_6D_6, 298 K): δ 38.8 ppm; ^{29}Si{^{1}H} NMR (99.3 MHz, C_6D_6, 298 K): δ 1.4 {s, LSiH(CH_2*Si*Me_3)=Si(TeBcat)($SiMe_3$)$_2$}, 0.30 {s, LSiH(CH_2SiMe_3)=Si(TeBcat)(*Si*Me_3)$_2$}, -2.7 {s, LSiH(CH_2SiMe_3)=*Si*(TeBcat)($SiMe_3$)$_2$}, -12.2 {s, L*Si*H(CH_2SiMe_3)=Si(TeBcat)($SiMe_3$)$_2$} ppm; ^{125}Te{^{1}H} NMR (126.3 MHz, C_6D_6, 298 K): δ -234.6 ppm. Due to the sensitivity of the compound we could not obtain a reliable elemental analysis data despite several attempts.

Representative NMR spectra:

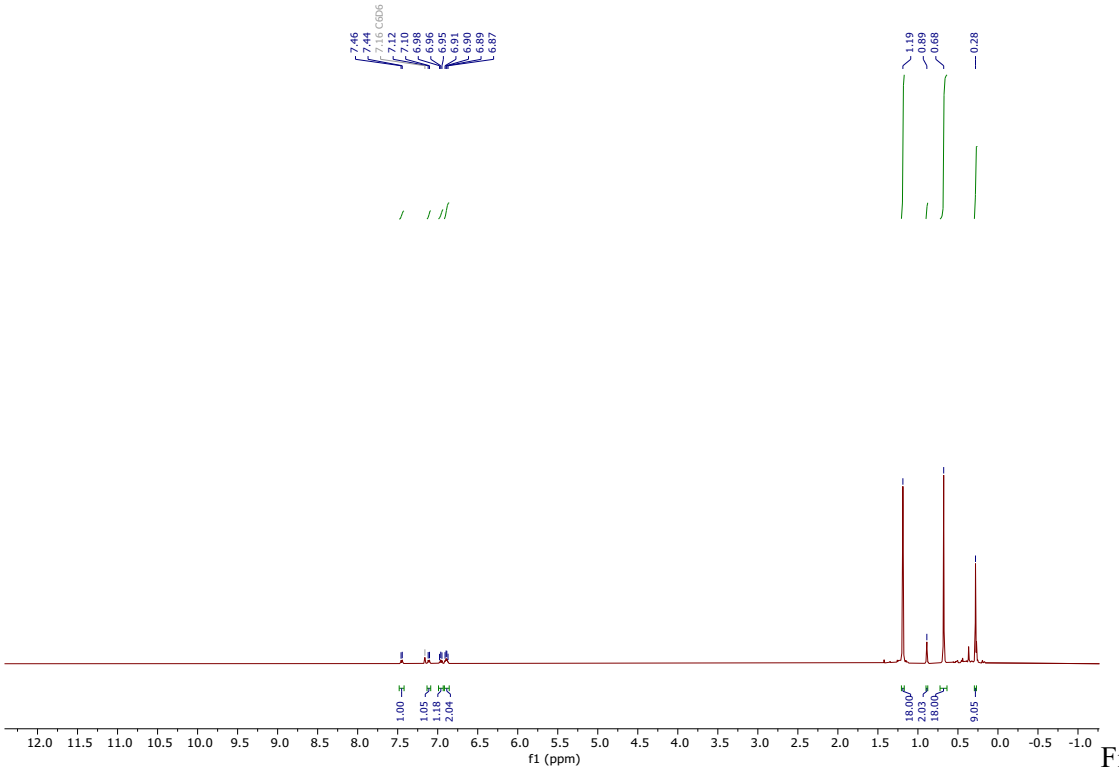


Figure S1. ^{1}H NMR Spectrum of **2** (C_6D_6, 400 MHz, 298 K)

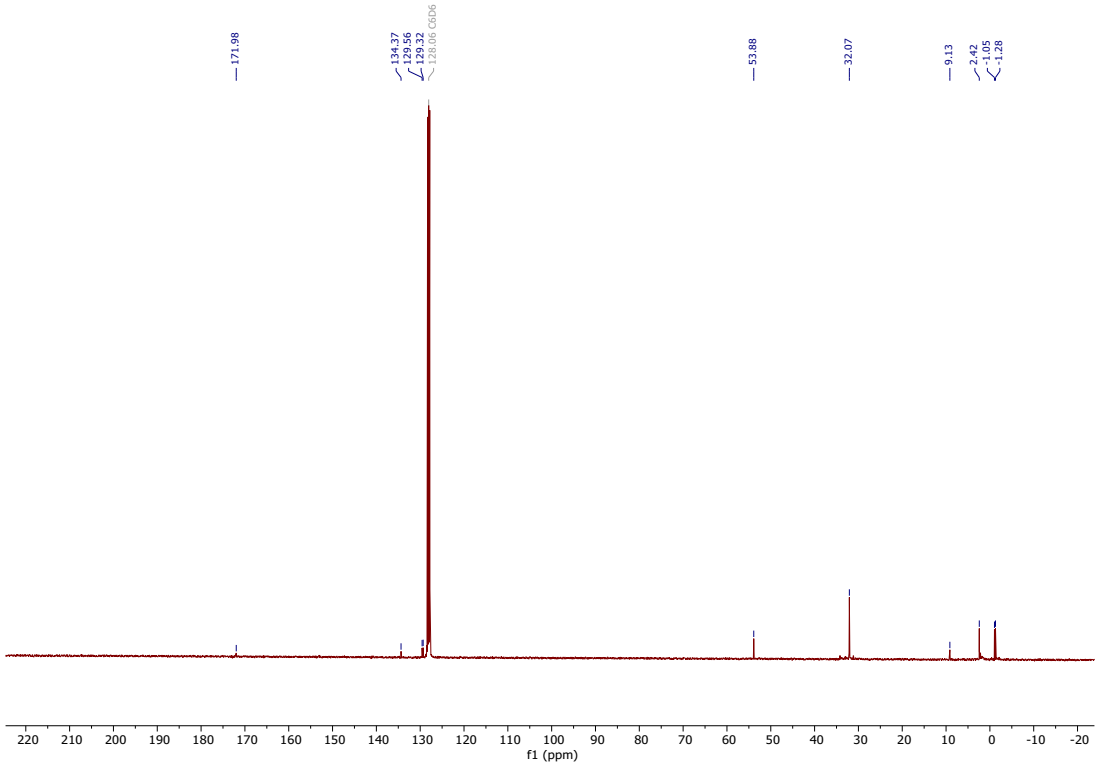


Figure S2. ^{13}C NMR Spectrum of **2** (C_6D_6, 100.6 MHz, 298 K)

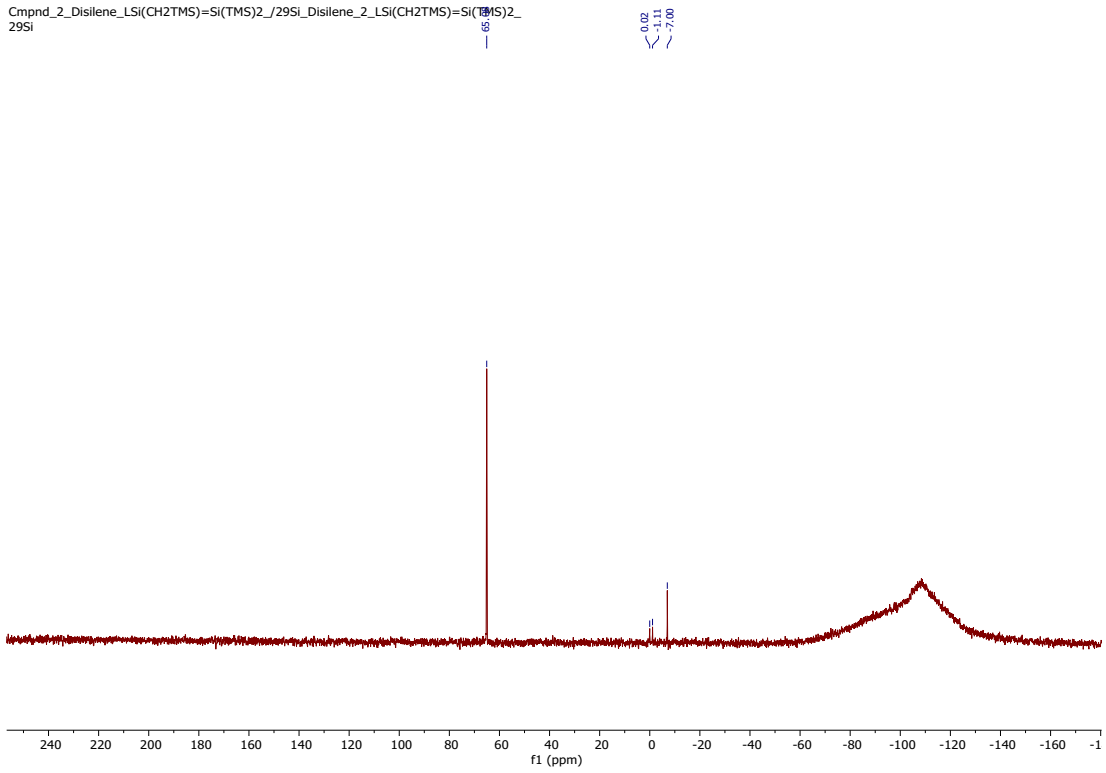


Figure S3. ^{29}Si NMR Spectrum of **2** (C_6D_6, 99.3 MHz, 298 K)

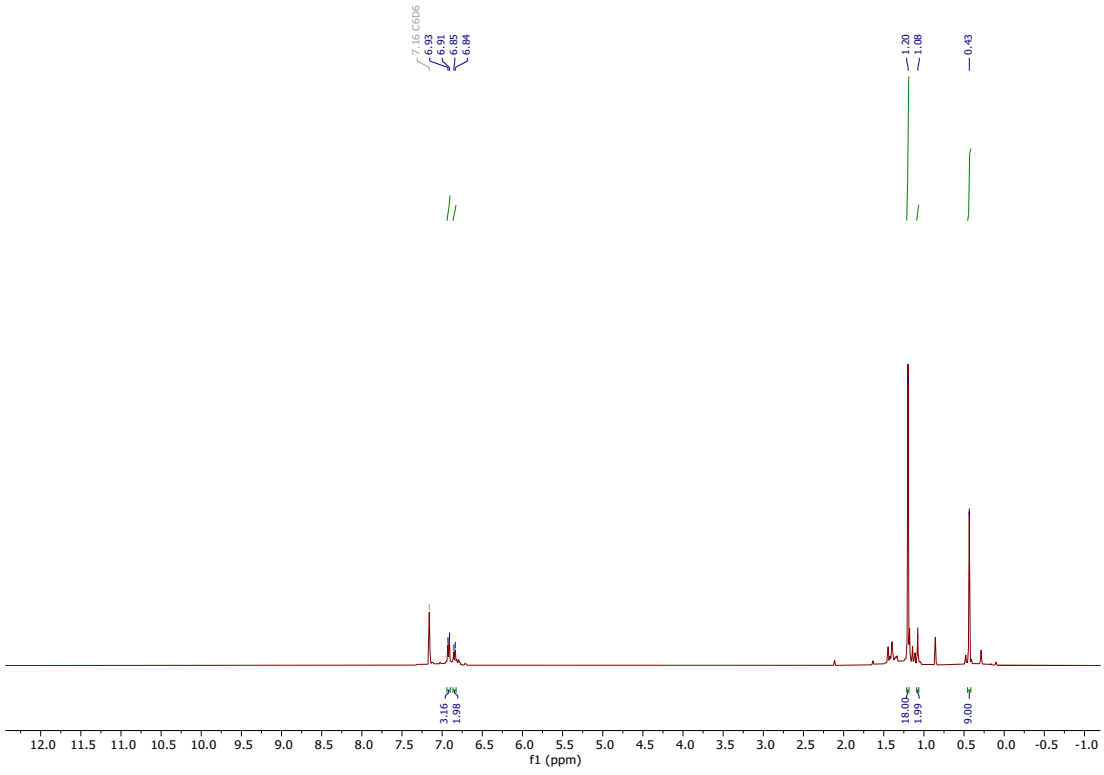


Figure S4. ^{1}H NMR Spectrum of **3** (C_6D_6, 500 MHz, 298 K)

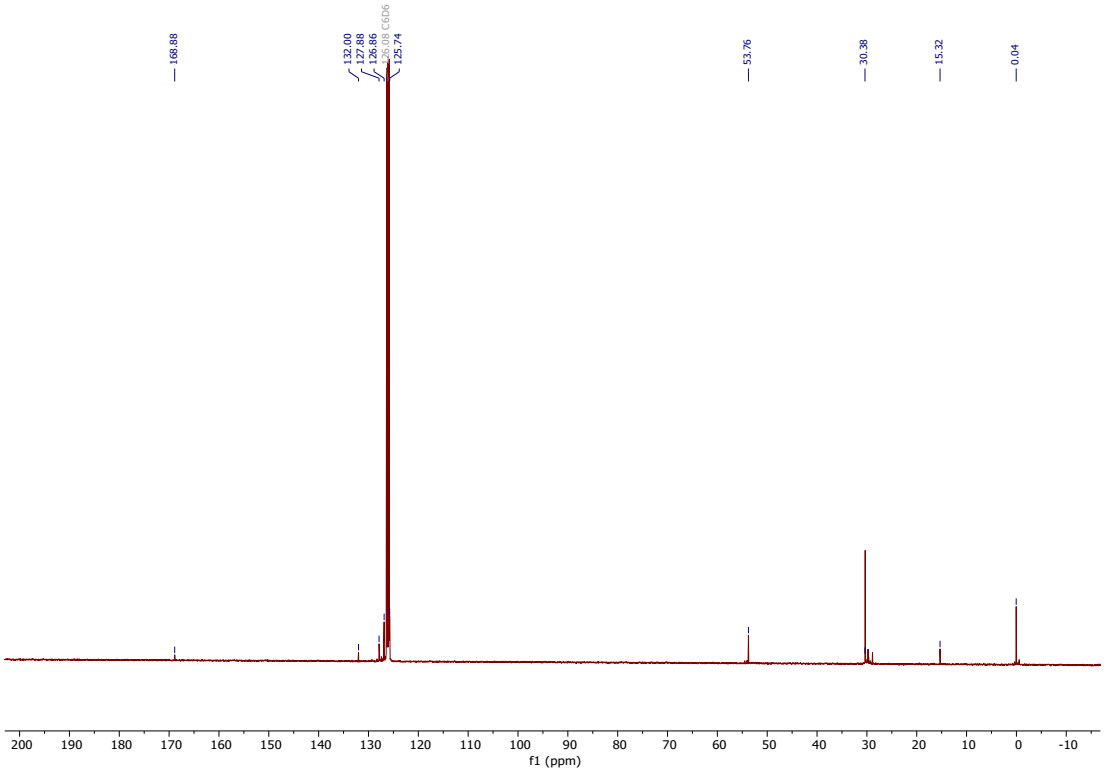


Figure S5. ^{13}C NMR Spectrum of **3** (C_6D_6, 125.7 MHz, 298 K)

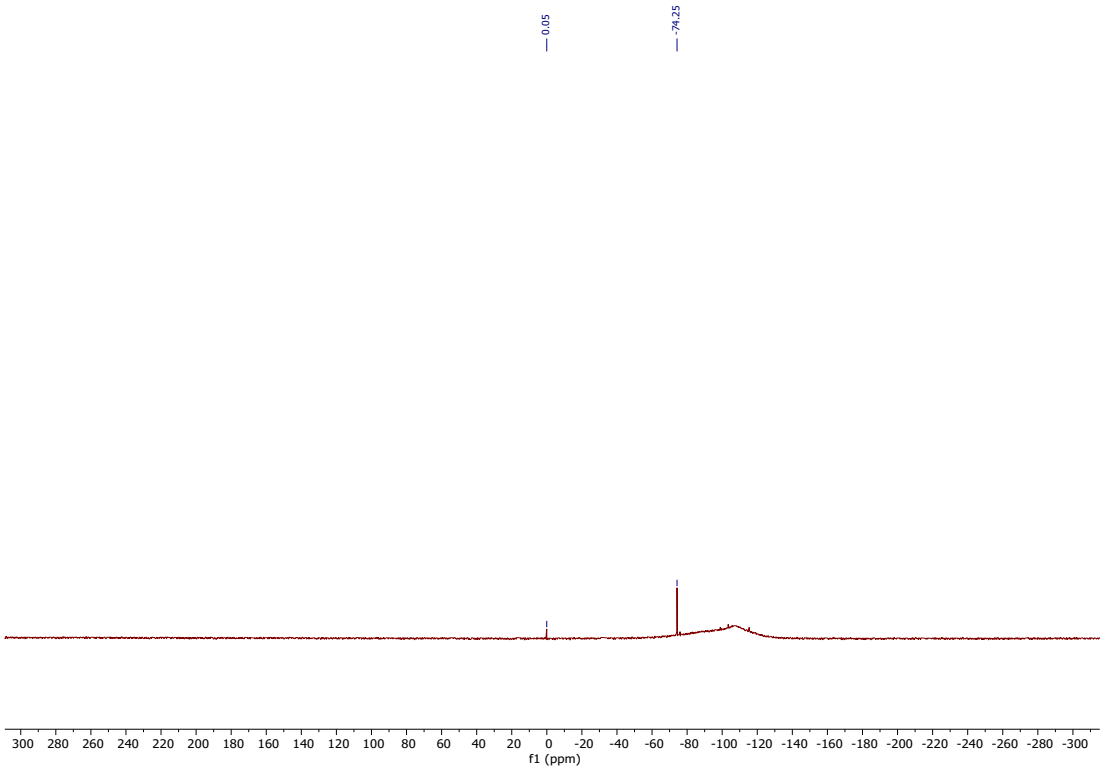


Figure S6. ^{29}Si NMR Spectrum of **3** (C_6D_6, 99.3 MHz, 298 K)

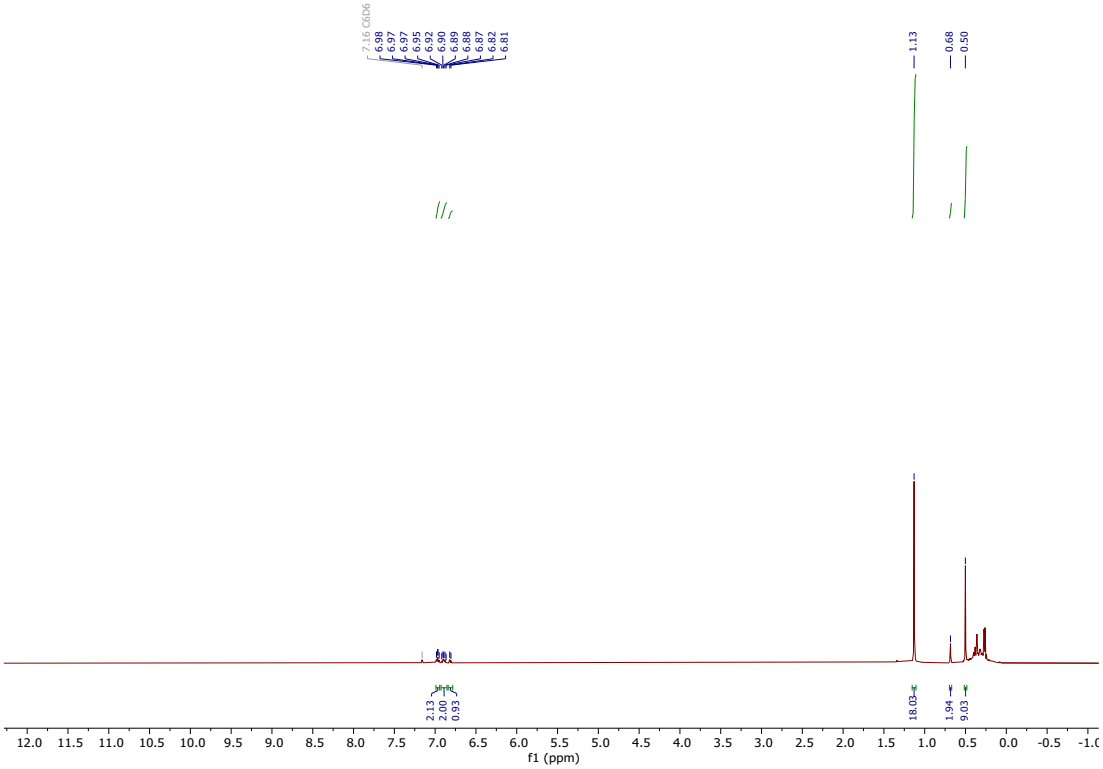


Figure S7. ^{1}H NMR Spectrum of **4** (C_6D_6, 400 MHz, 298 K)

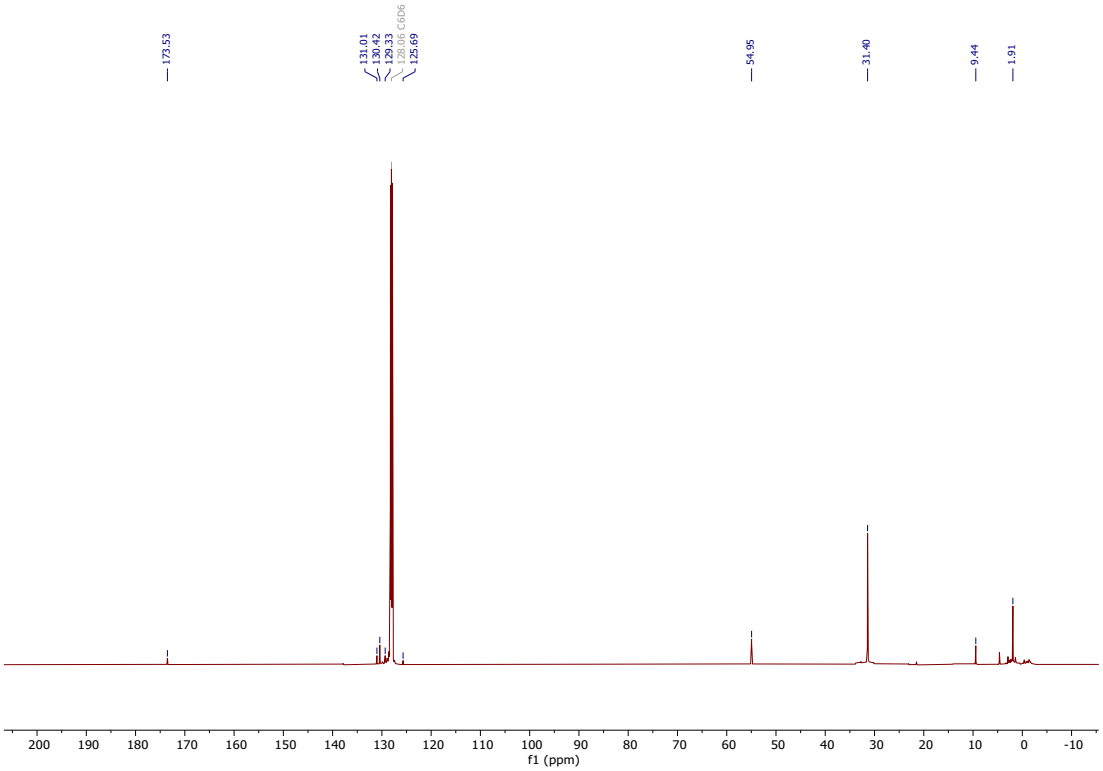


Figure S8. ^{13}C NMR Spectrum of **4** (C_6D_6, 100.6 MHz, 298 K)

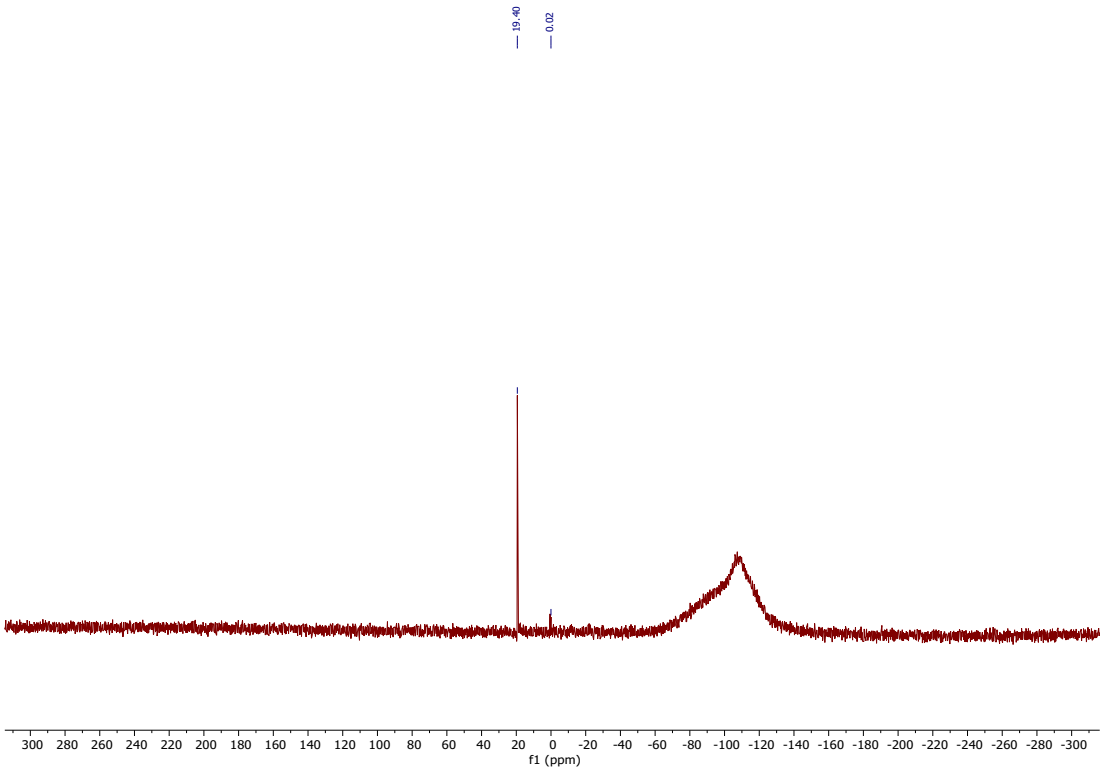


Figure S9. ^{29}Si NMR Spectrum of **4** (C_6D_6, 99.3 MHz, 298 K)

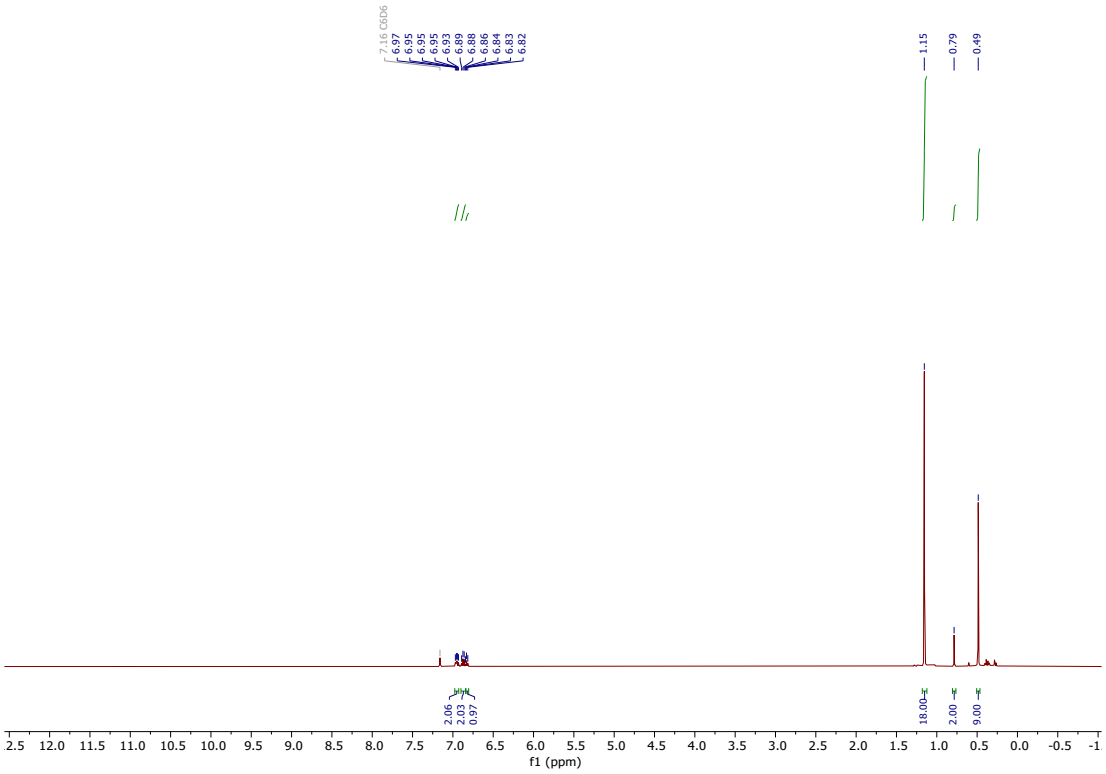
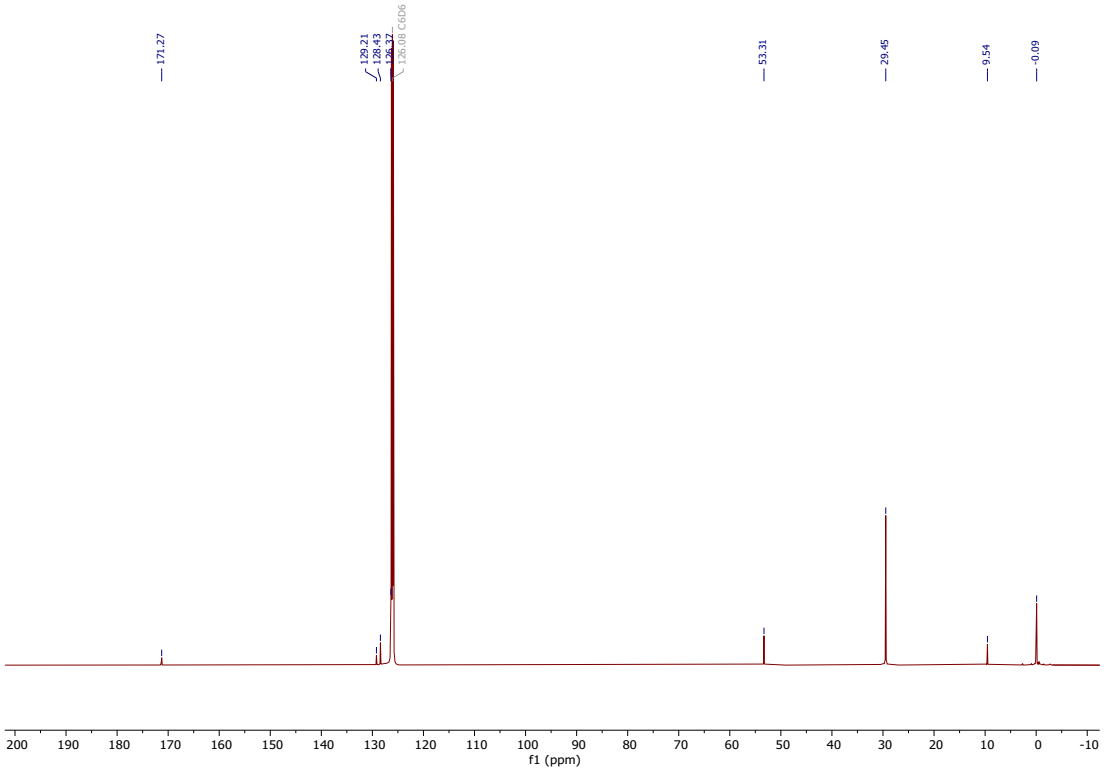


Figure S10. ^{1}H NMR Spectrum of **5** (C_6D_6, 400 MHz, 298 K)



S11. ^{13}C NMR Spectrum of **5** (C_6D_6, 100.6 MHz, 298 K)

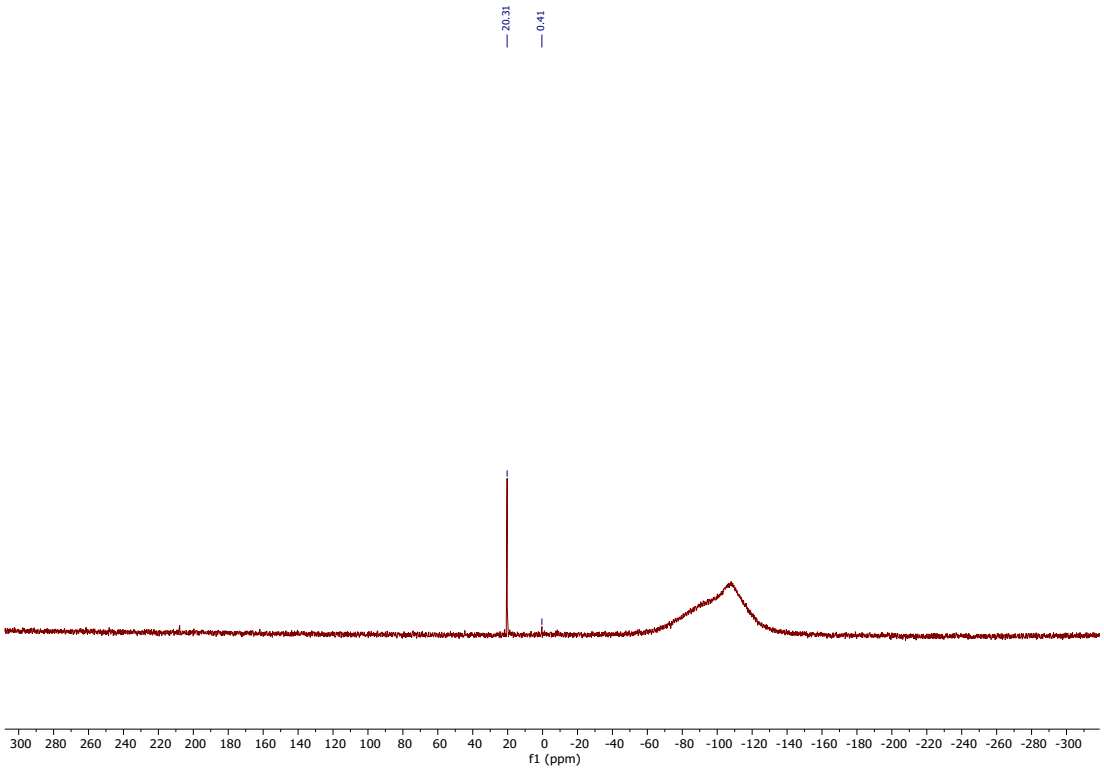


Figure S12. ^{29}Si NMR Spectrum of **5** (C_6D_6, 99.3 MHz, 298 K)

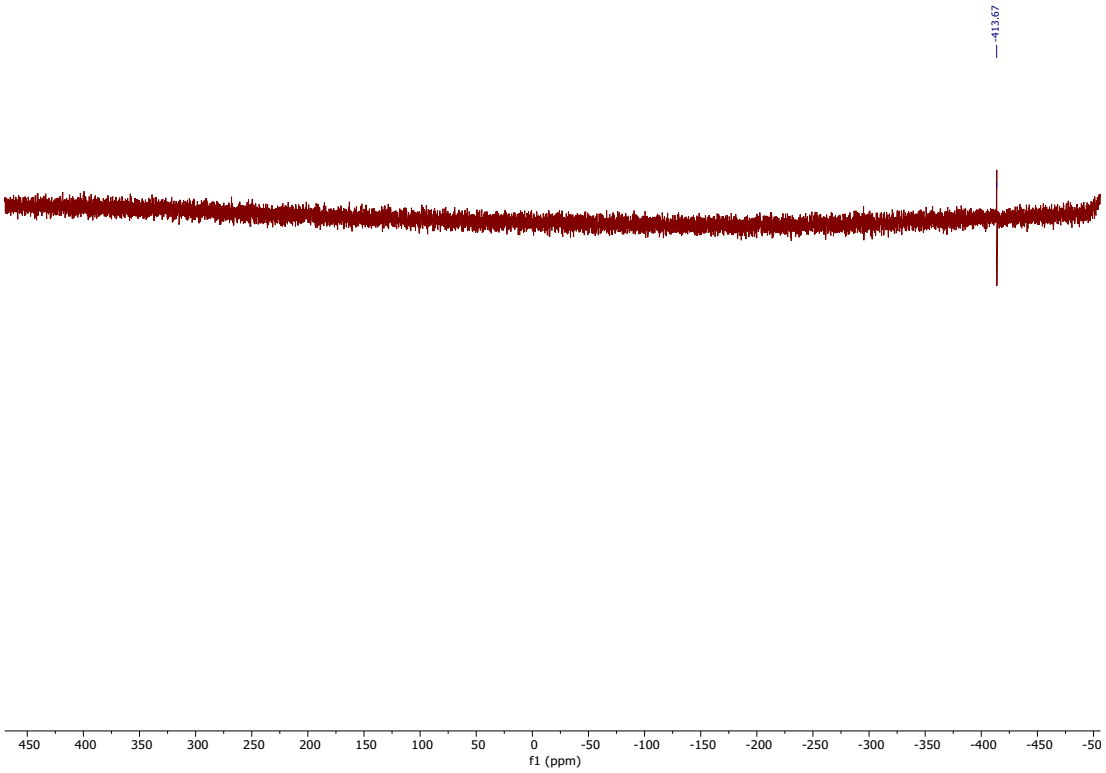


Figure S13. ^{77}Se NMR Spectrum of **5** (C_6D_6, 76.3 MHz, 298 K)

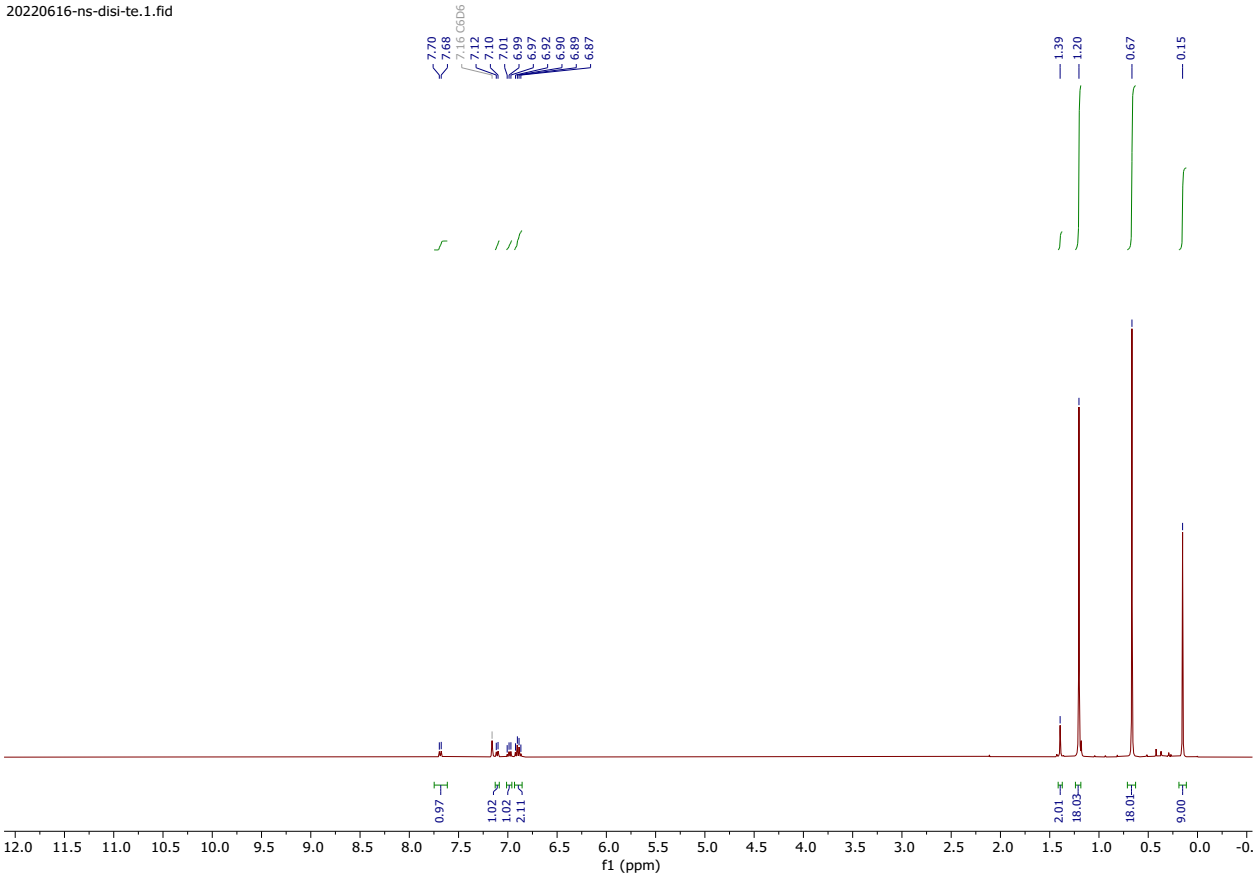
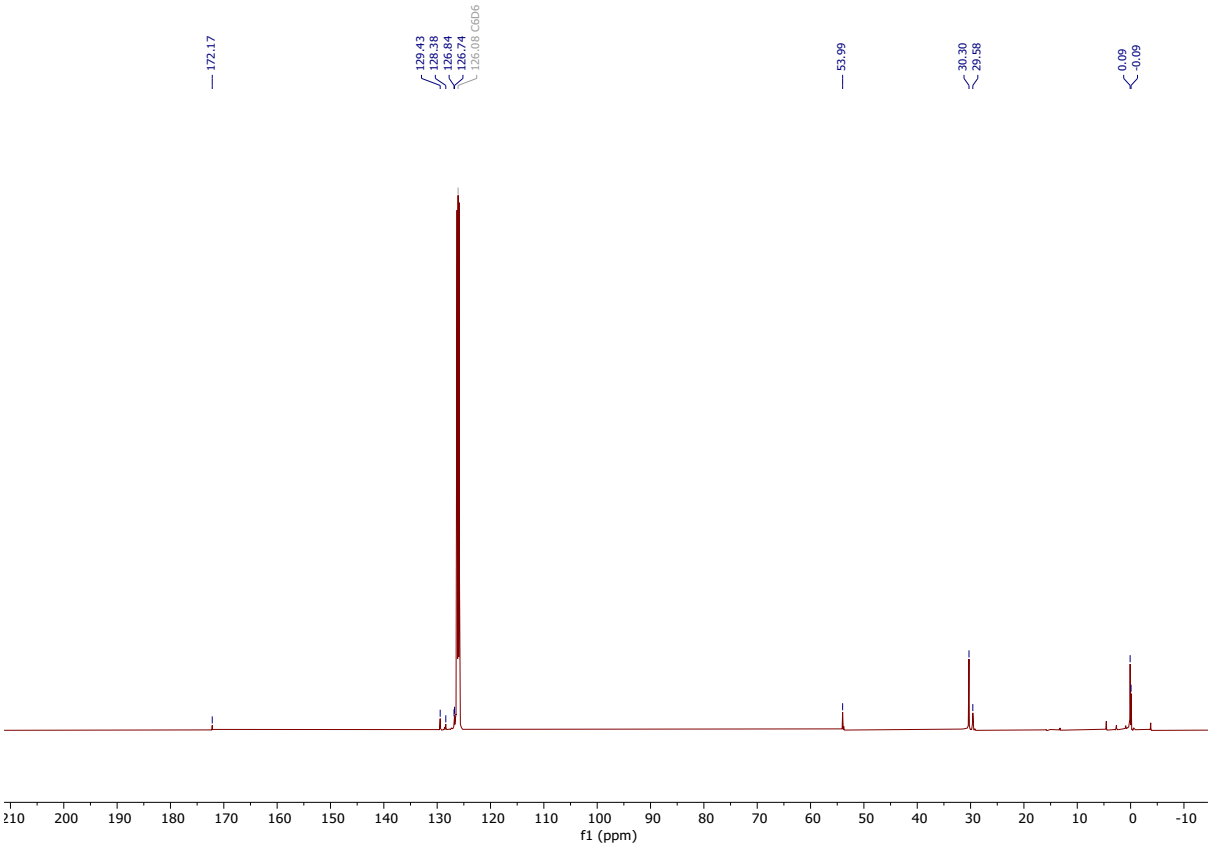


Figure S14. ^{1}H NMR Spectrum of **6** (C_6D_6, 400 MHz, 298 K)



S15. ^{13}C NMR Spectrum of **6** (C_6D_6, 100.6 MHz, 298 K)

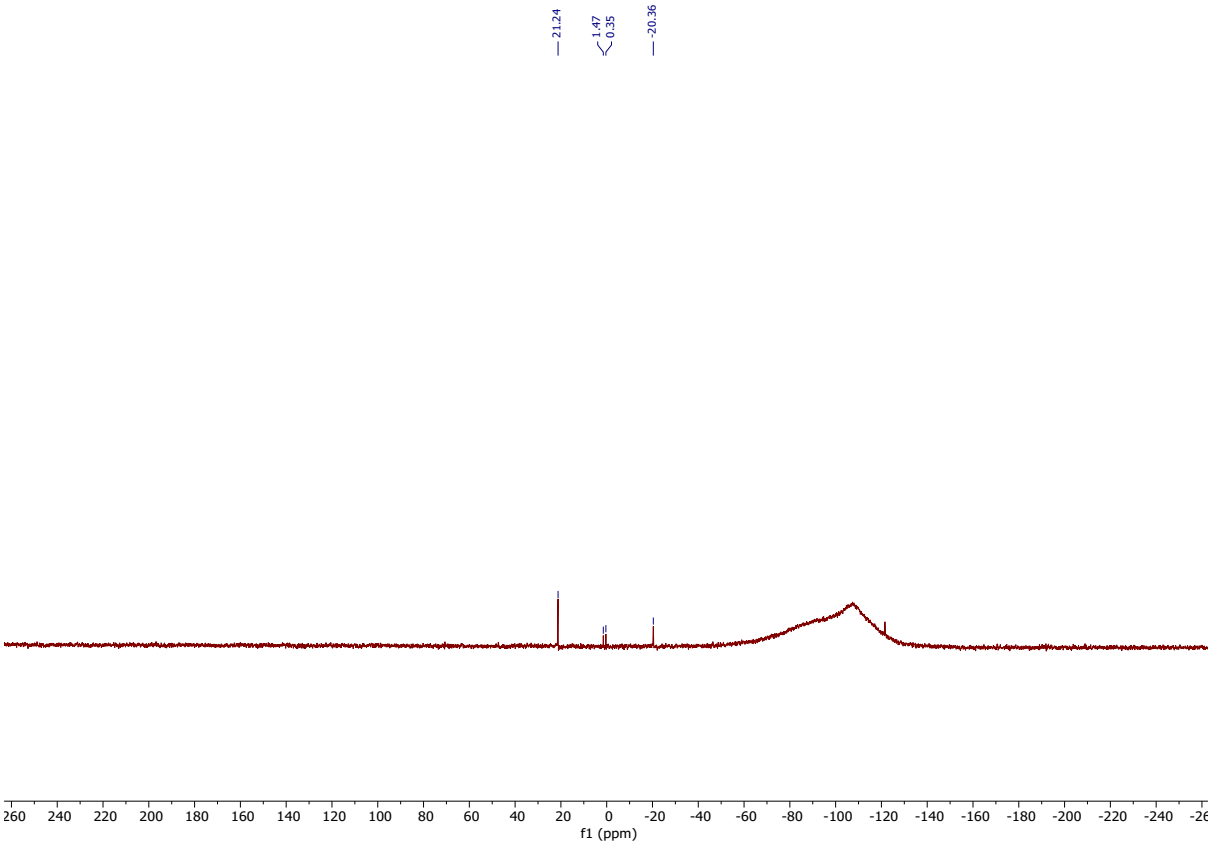


Figure S16. ^{29}Si NMR Spectrum of **6** (C_6D_6, 99.3 MHz, 298 K)

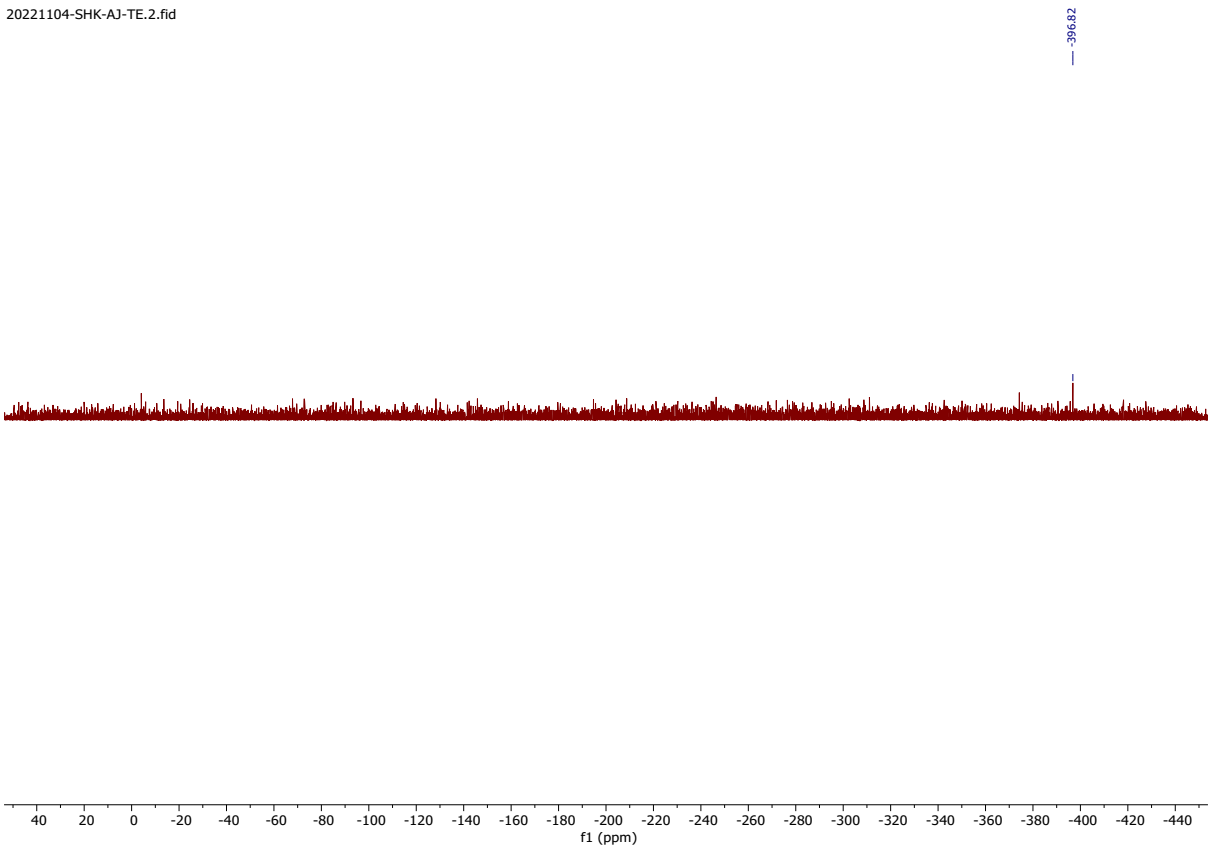


Figure S17. ^{125}Te NMR Spectrum of **6** (C_6D_6, 126.3 MHz, 298 K).

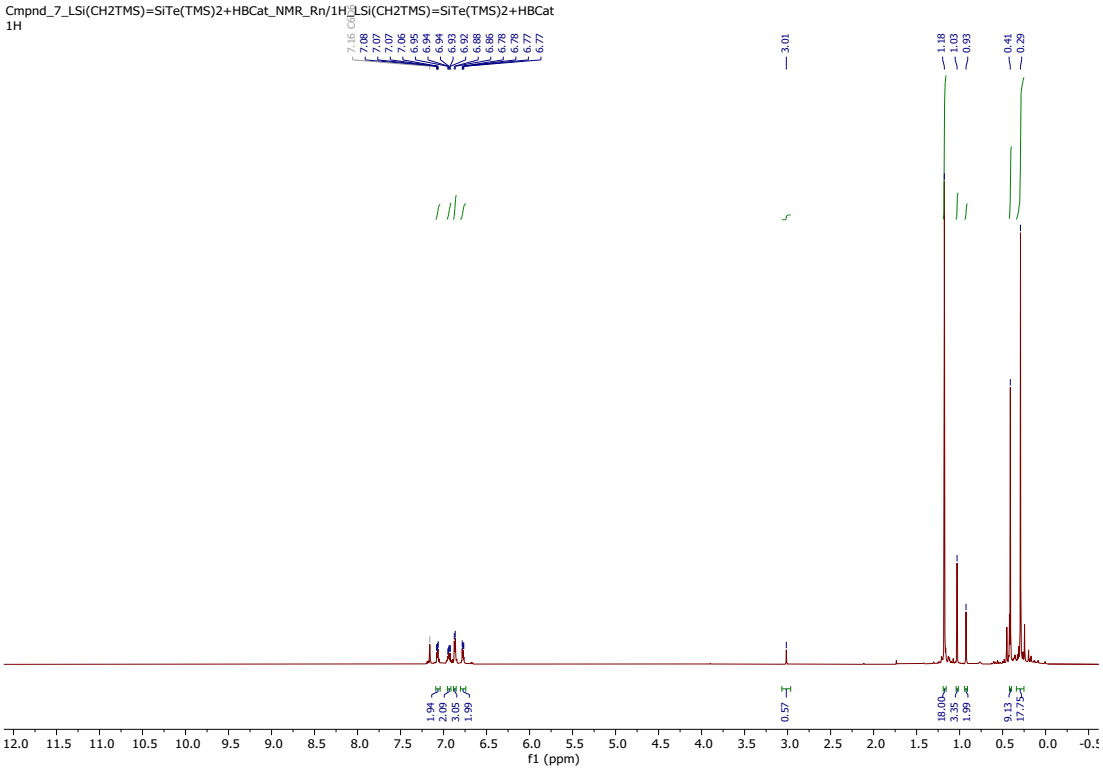


Figure S18. ^{1}H NMR Spectrum of **6** + HBcat reaction (C_6D_6, 400 MHz, 298 K)

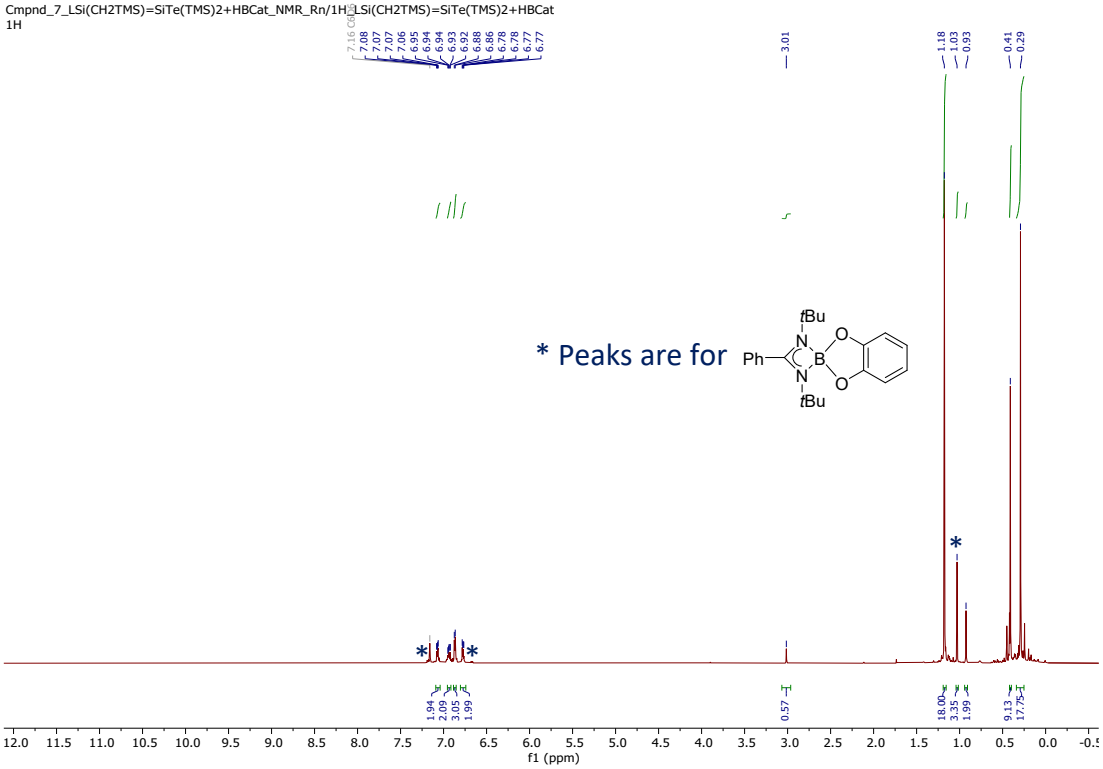


Figure S19. ^{1}H NMR Spectrum of **6** + HBcat reaction (C_6D_6, 400 MHz, 298 K)

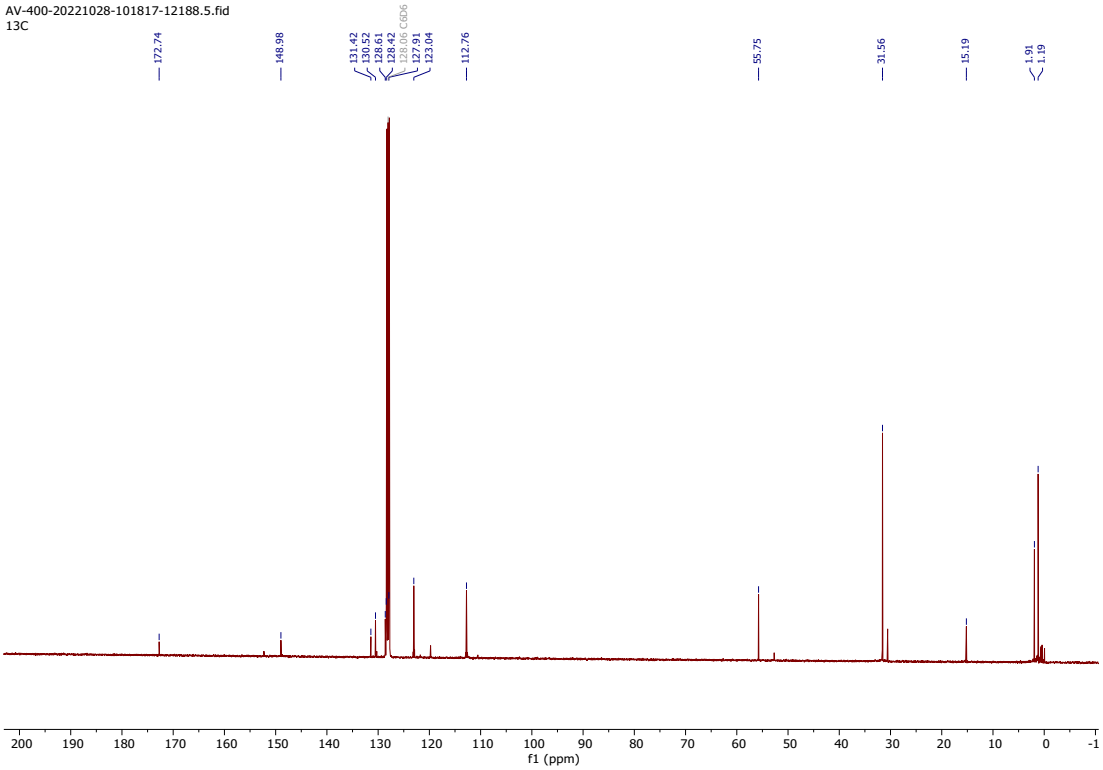


Figure S20. ^{13}C NMR Spectrum of **6** + HBcat reaction (C_6D_6, 100.6 MHz, 298 K)

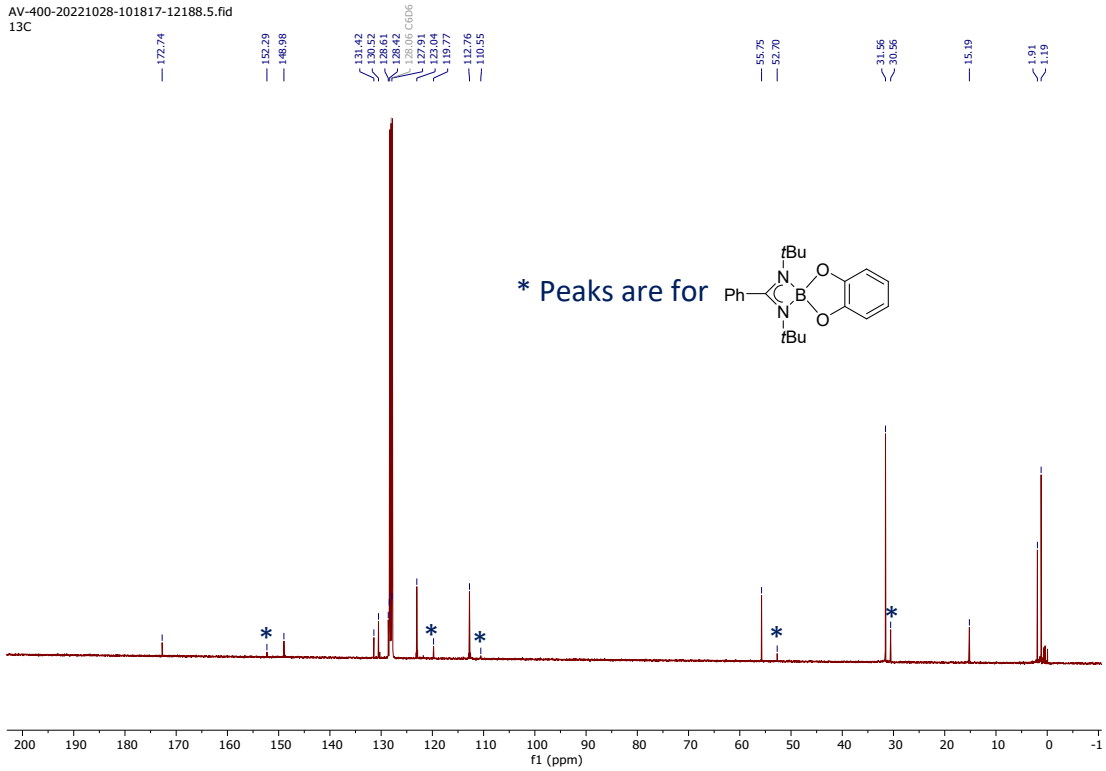


Figure S21. ^{13}C NMR Spectrum of **6** + HBcat reaction (C_6D_6, 100.6 MHz, 298 K)

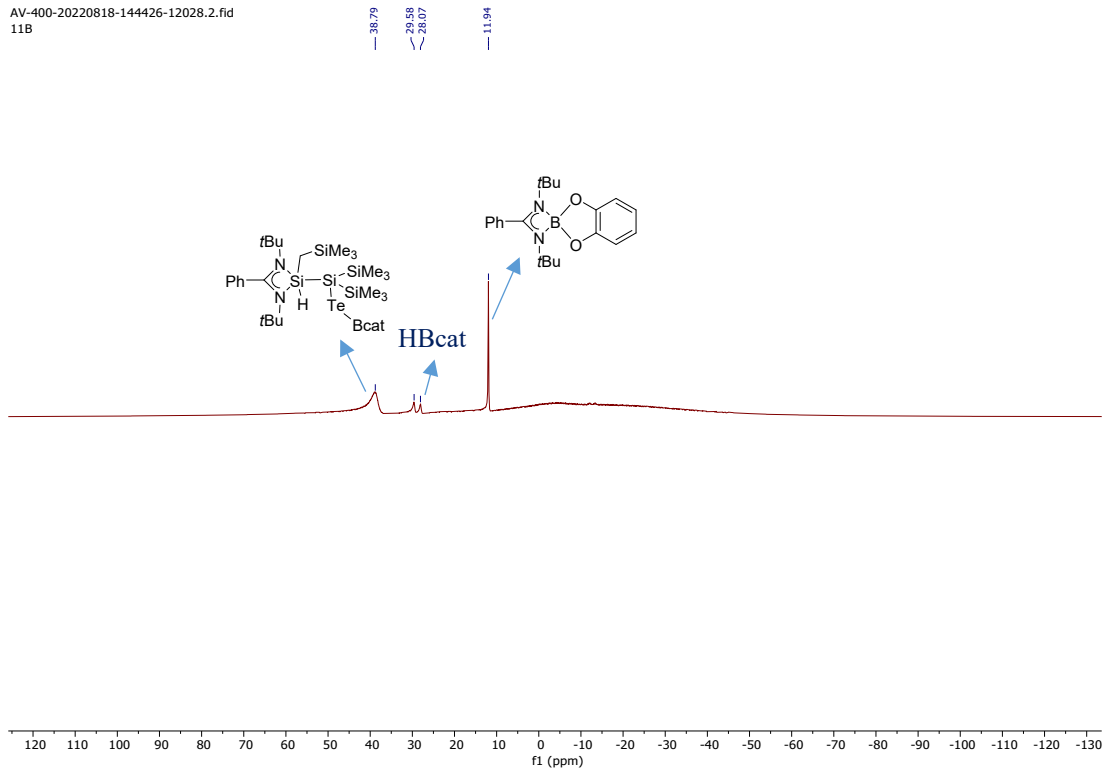


Figure S22. ^{11}B NMR Spectrum of **6** + HBcat reaction (C_6D_6, 128.3 MHz, 298 K)

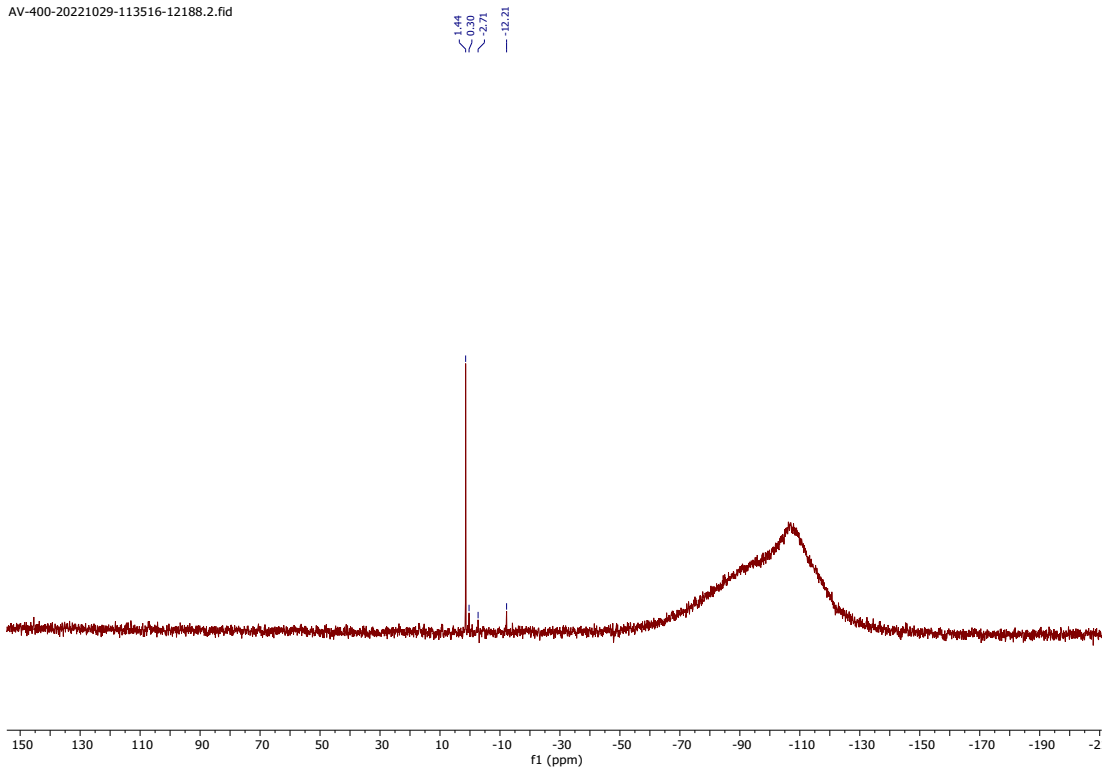


Figure S23. ^{29}Si NMR Spectrum of **6** + HBcat reaction (C_6D_6, 99.3 MHz, 298 K)

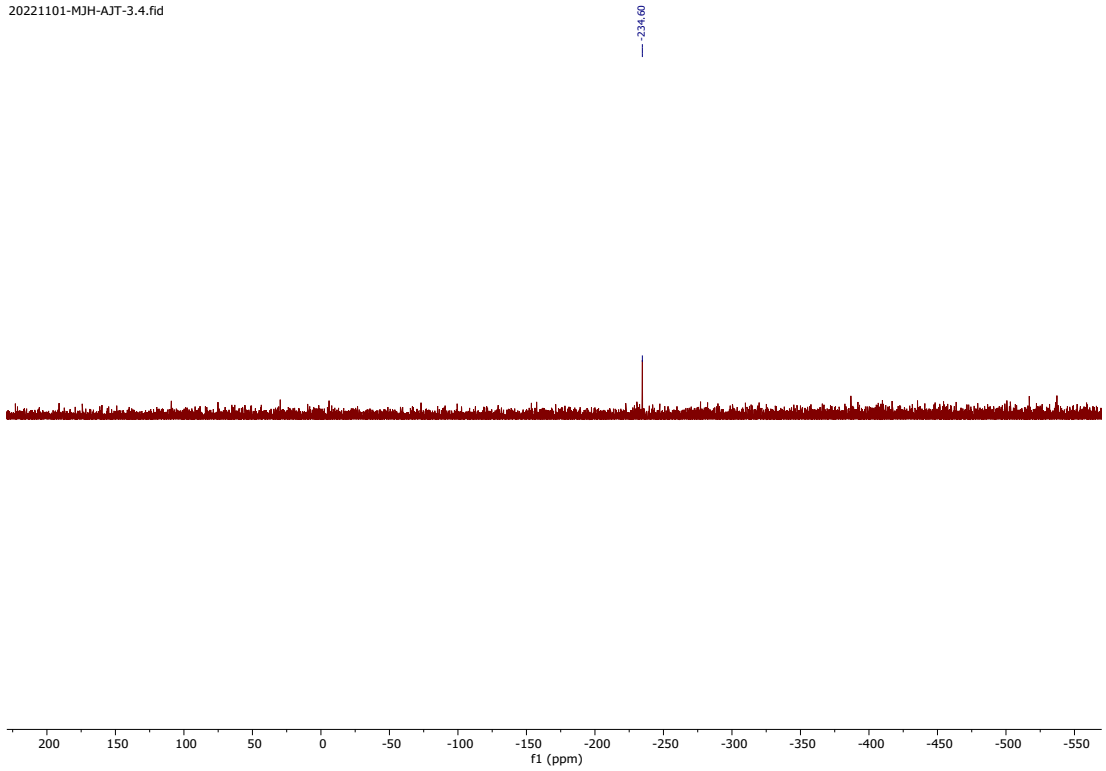


Figure S24. ^{125}Te NMR Spectrum of **6** + HBcat reaction (C_6D_6, 126.3 MHz, 298 K)

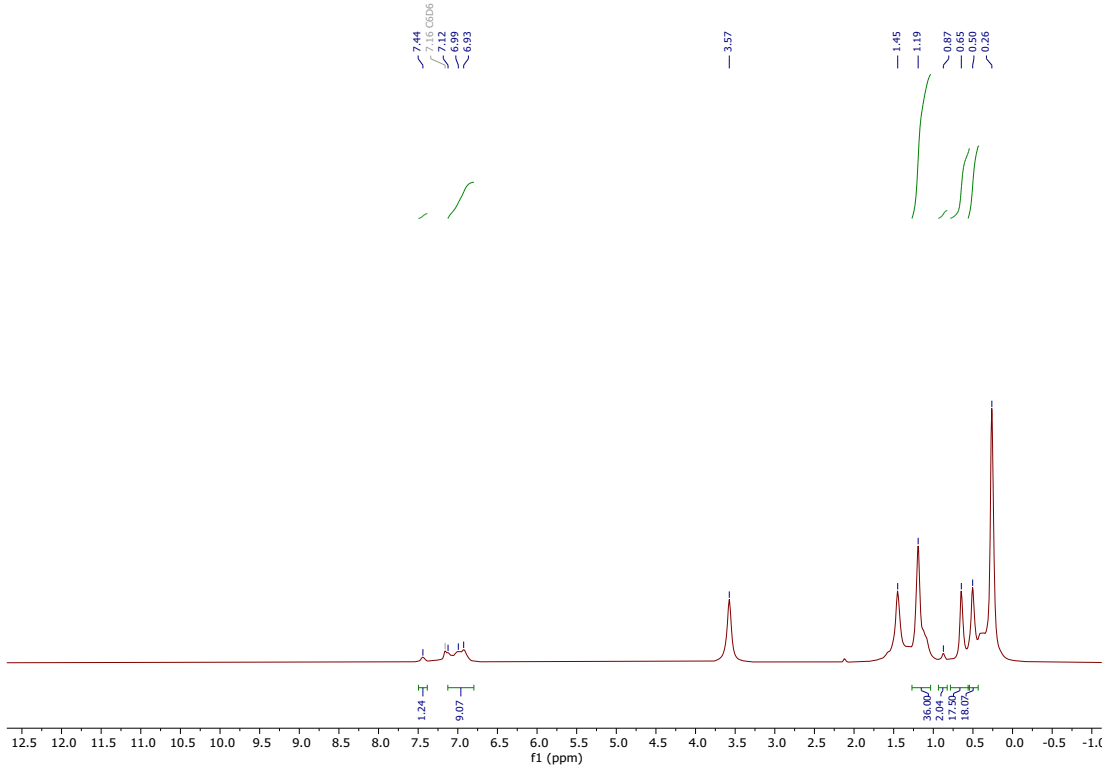


Figure S25. ^{1}H NMR Spectrum for the NMR tube reaction of **3** and $KSi(SiMe_3)_3$. 2thf (C_6D_6, 400 MHz, 298 K)

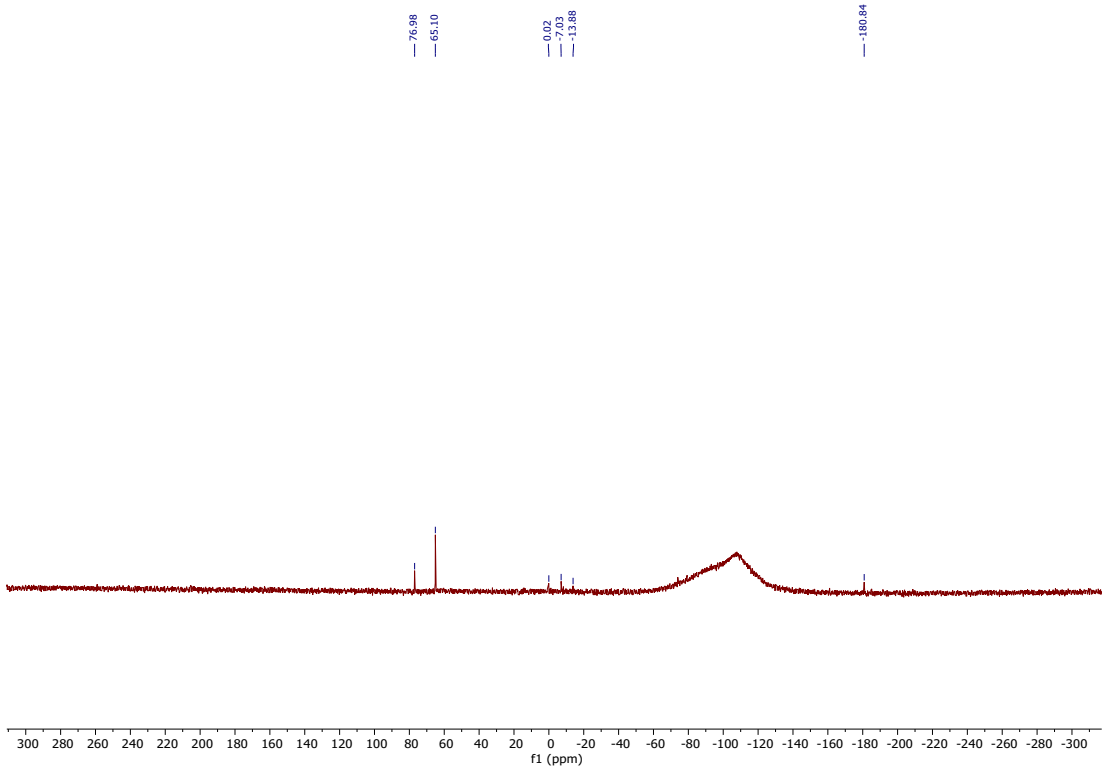


Figure S26. ^{29}Si NMR Spectrum for the NMR tube reaction of **3** and $KSi(SiMe_3)_3$. 2thf (C_6D_6, 99.3 MHz, 298 K)

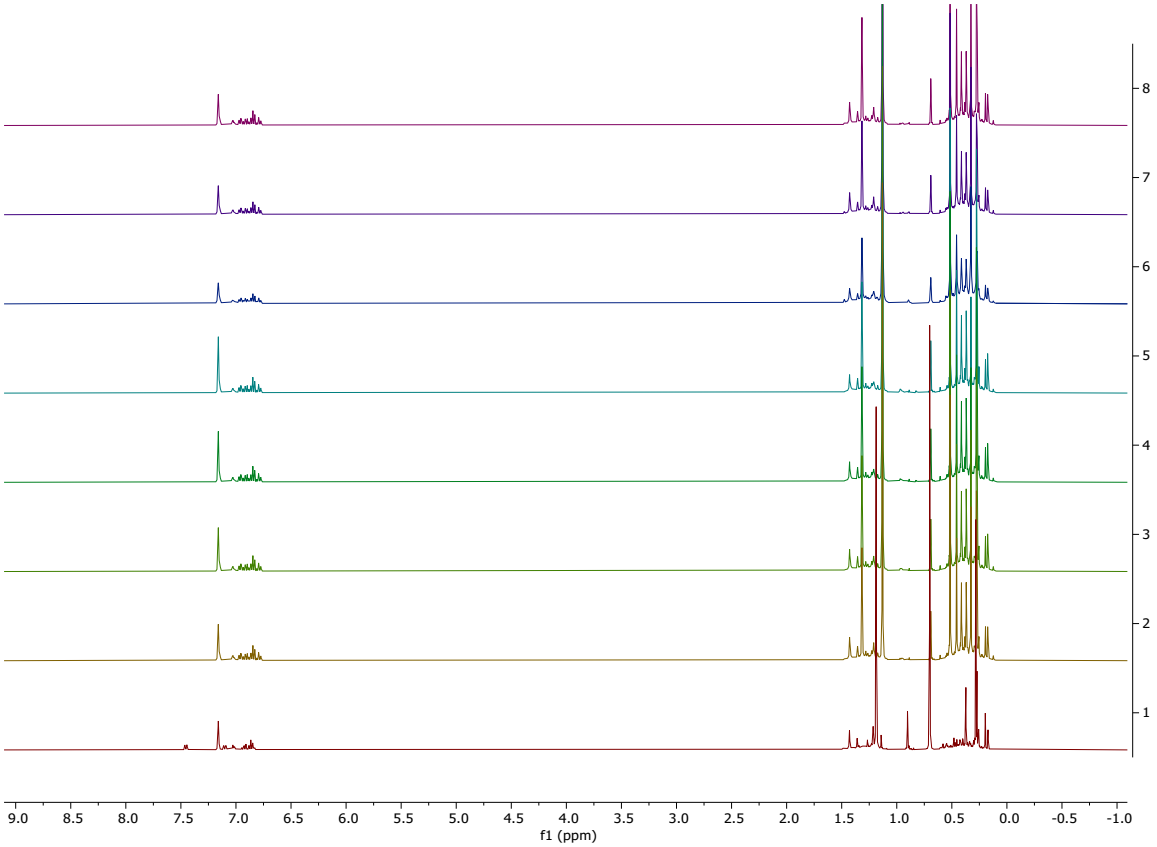


Figure S27. Stacked NMR for the reaction of **2** and S (Stacked NMR No. 1 is for pure disilene (**2**), and NMR No. 2 to 8 were taken in time interval of six minutes).

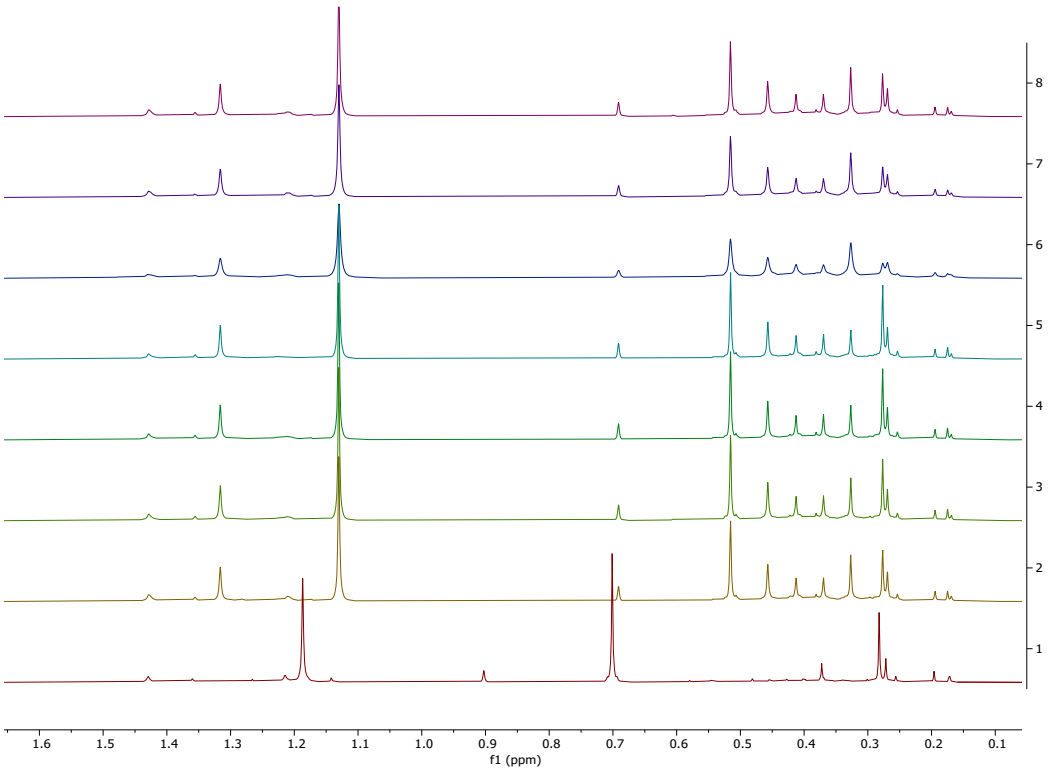


Figure S28. Cropped portion of the stacked NMR for the reaction of **2** and S (Stacked NMR No. 1 is for pure disilene (**2**), and NMR No. 2 to 8 were taken in time interval of six minutes).

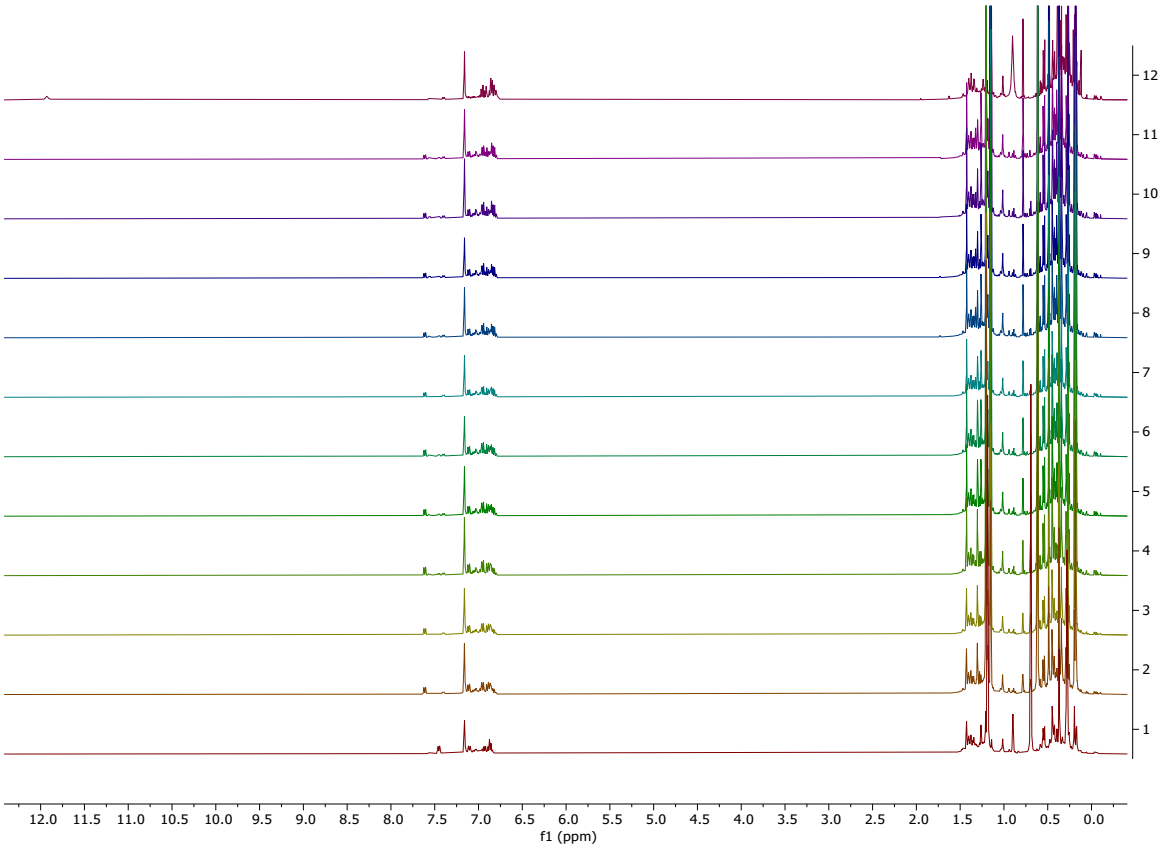


Figure S29. Stacked NMR for the reaction of **2** and Se (Stacked NMR No. 1 is for pure disilene (**2**), and NMR No. 2 to 11 were taken in time interval of six minutes, and NMR No. 12 was taken after 12 h).

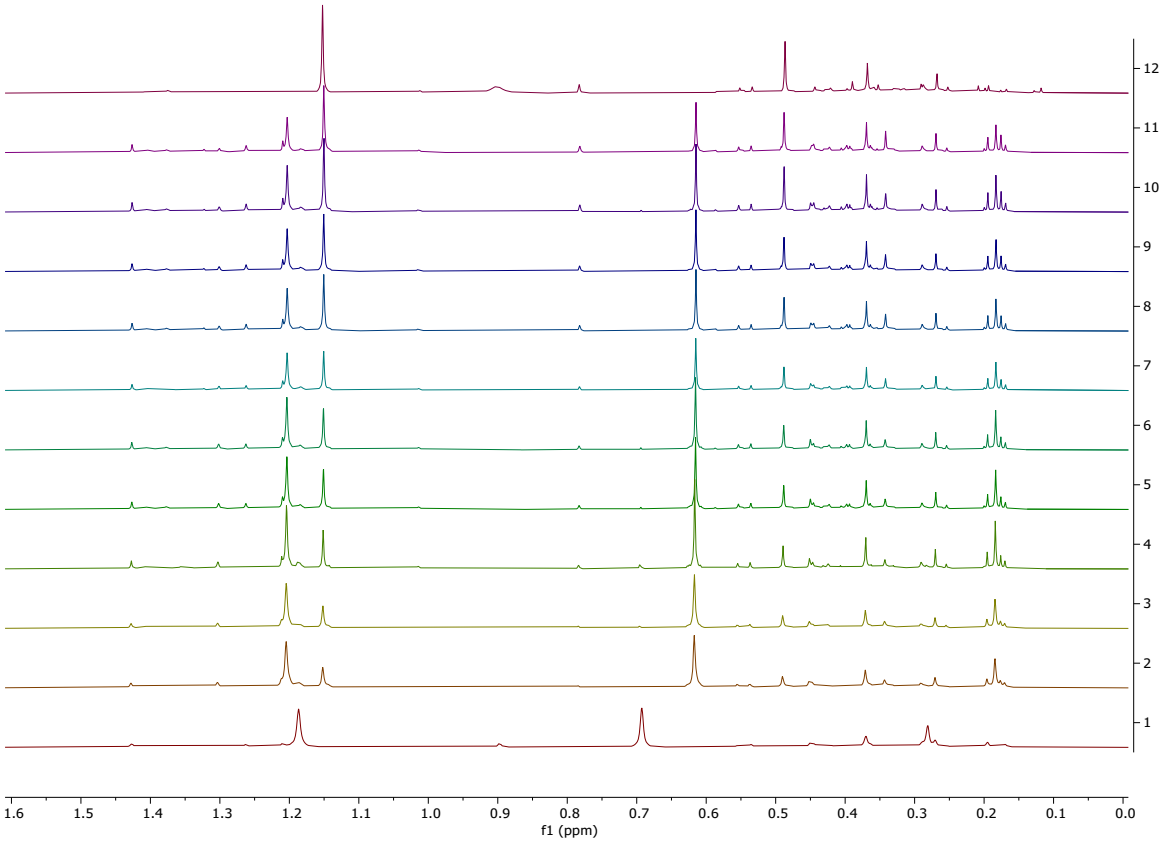


Figure S30. Cropped portion of the stacked NMR for the reaction of **2** and Se (Stacked NMR No. 1 is for pure disilene (**2**), and NMR No. 2 to 11 were taken in time interval of six minutes, and NMR No. 12 was taken after 12 h).

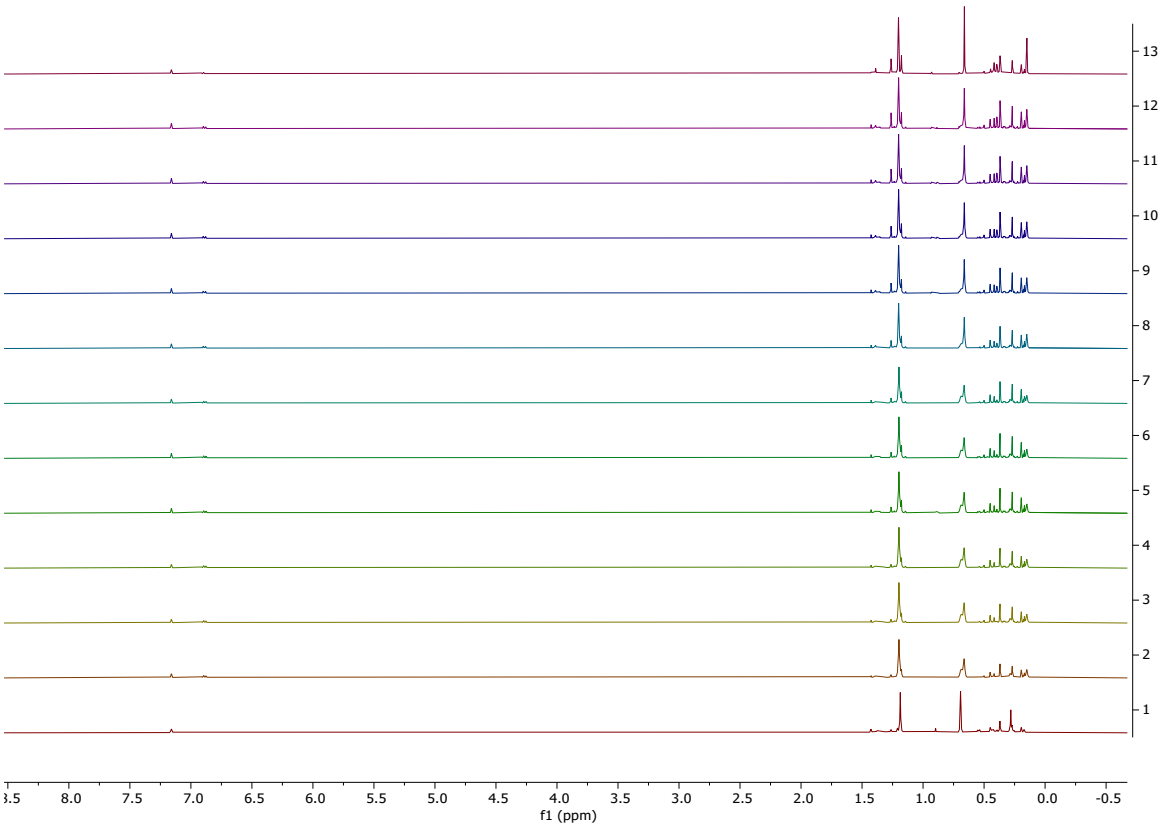


Figure S31. Stacked NMR for the reaction of **2** and Te (Stacked NMR No. 1 is for pure disilene (**2**), and NMR No. 2 to 12 were taken in time interval of six minutes, and NMR No. 13 was taken after 12 h).

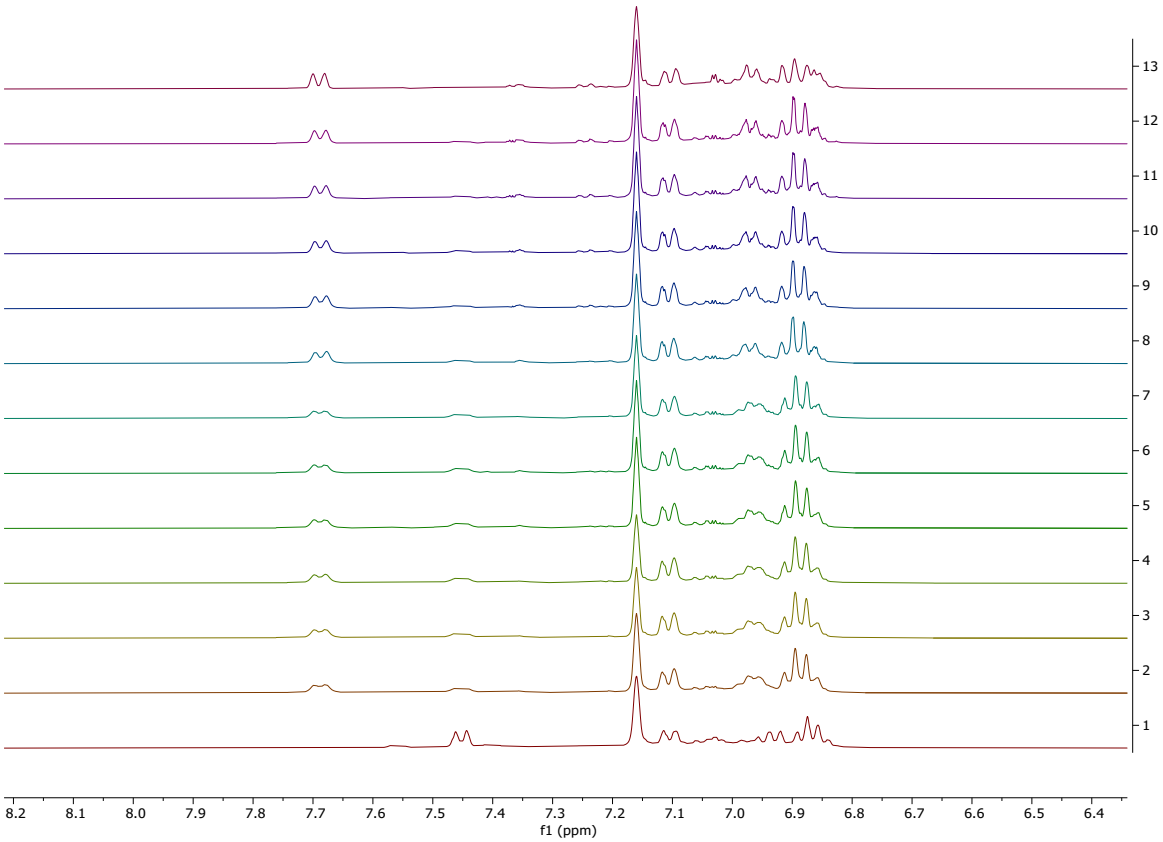


Figure S32. Cropped portion of the stacked NMR for the reaction of **2** and Te (Stacked NMR No. 1 is for pure disilene (**2**), and NMR No. 2 to 12 were taken in time interval of six minutes, and NMR No. 13 was taken after 12 h).

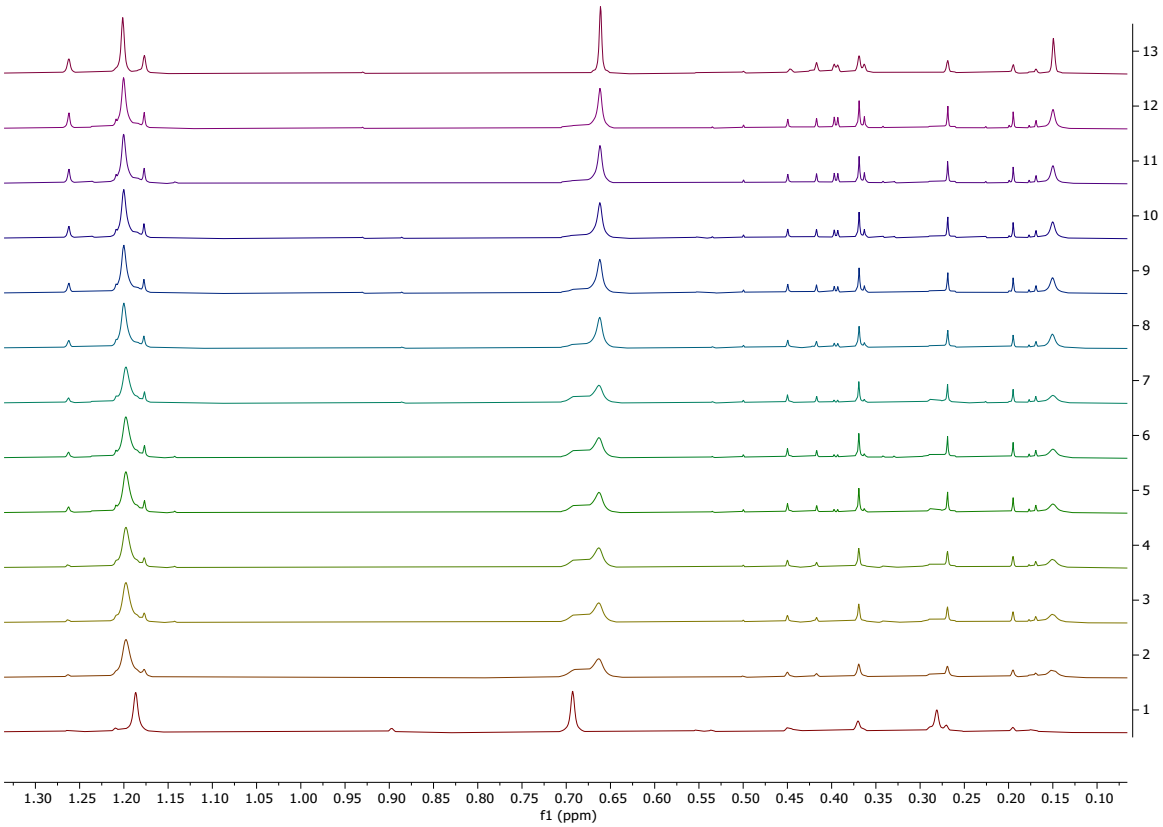


Figure S33. Cropped portion of the stacked NMR for the reaction of **2** and Te (Stacked NMR No. 1 is for pure disilene (**2**), and NMR No. 2 to 12 were taken in time interval of six minutes, and NMR No. 13 was taken after 12 h).

Computational Details

All the calculations in this study have been performed with density functional theory (DFT), with the aid of the Turbomole 7.5 suite of programs,[4] using the PBE functional,[5] along with dispersion correction (DFT-D3)[6]. The def2-TZVP basis set[7] has been employed. The resolution of identity (RI),[8] along with the multipole accelerated resolution of identity (marij)[9] approximations have been employed for an accurate and efficient treatment of the electronic Coulomb term in the DFT calculations. Solvent corrections were incorporated with optimization calculations using the COSMO model,[10] with toluene (ε = 2.374) as the solvent. The values reported are ΔG values, with zero-point energy corrections, internal energy and entropic contributions included through frequency calculations on the optimized minima, with the temperature taken to be 298.15 K. Harmonic frequency calculations were performed for all stationary points to confirm them as local minima or transition state structures. For accurate HOMO-LUMO energy gap values, we have optimized the geometries of compounds **2** and **6** at the B3LYP/6-31g(d) level of theory[11] using the Gaussian 09 suite of programs.[12] Furthermore, NBO calculations[13] have been done at the B3LYP/6-31g(d)//B3-LYP/6-311+g(d) level of theory. For both optimization and single-point calculations, we have employed an implicit solvent model (PCM, toluene as solvent).[14]

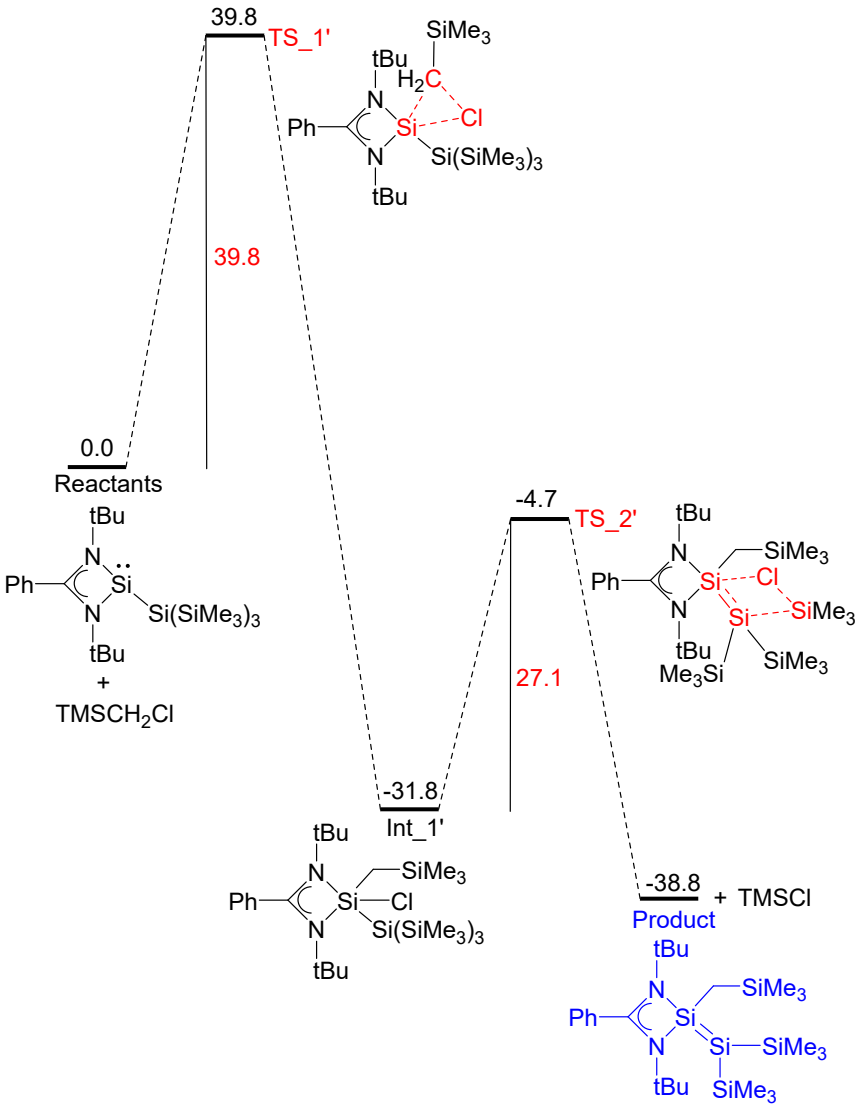


Figure S34. The free energy profile for the formation of **2**. Values are in kcal/mol.

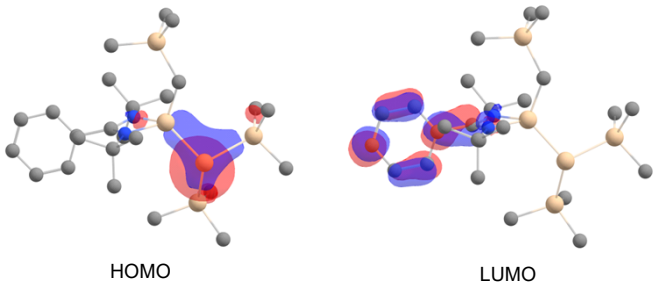


Figure S35. The HOMO and LUMO of **2** (with an iso-surface value of 0.05 a.u.).

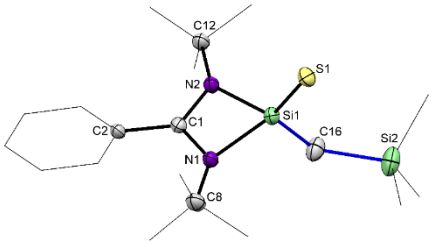


Figure S36. The molecular structure of **4**. Anisotropic displacement parameters are depicted at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and bond angles (deg): Si1-S1 1.9828(10), Si1-C16 1.861(3), Si2-C16 1.861(3); S1-Si1-C16 120.31(9), Si1-C16-Si2 120.80(15), N1-Si1-S1 117.85(8), N2-Si1-C16 107.62(11).

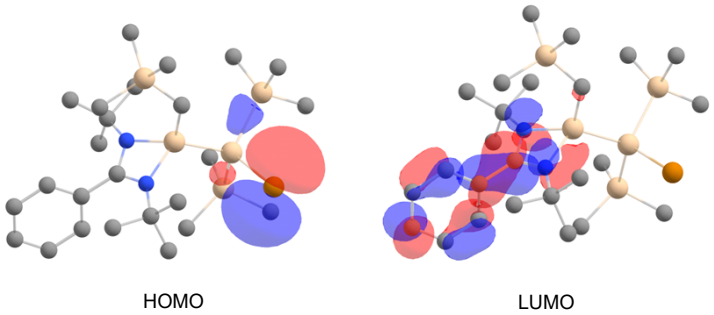


Figure S37. The HOMO and LUMO of **6** (with an iso-surface value of 0.04 a.u.).

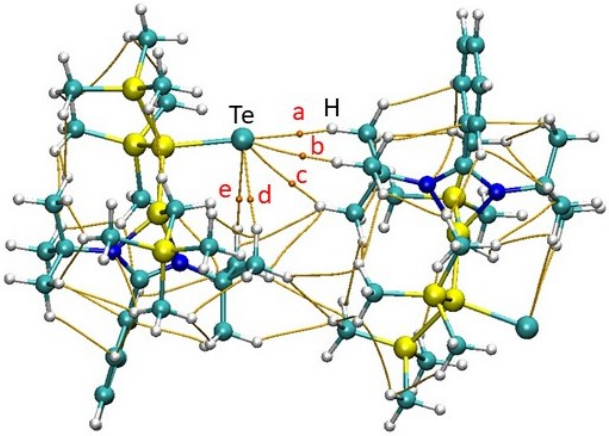


Figure S38. The bond critical points (a-e) for the inter- and intramolecular CH•••Te interactions. For clarity, other bond critical points have been omitted.

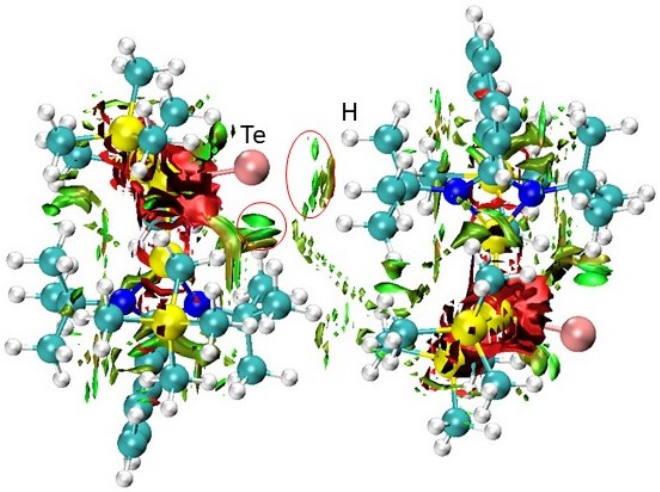
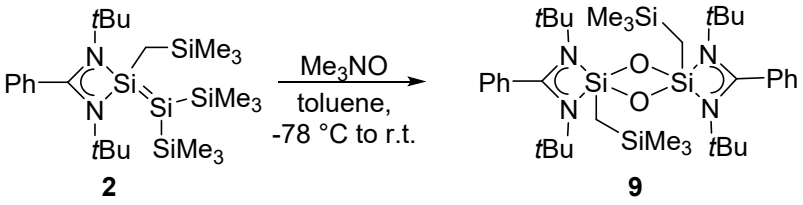


Figure S39. The NCI plot for the CH---Te interactions in the dimer. The red circles mark the isosurfaces corresponding to the inter- and intramolecular CH---Te interactions. In the NCI plot, blue, green, and red represent strong attraction, weak attraction, and strong repulsion, respectively.

Reaction with Me_3NO.



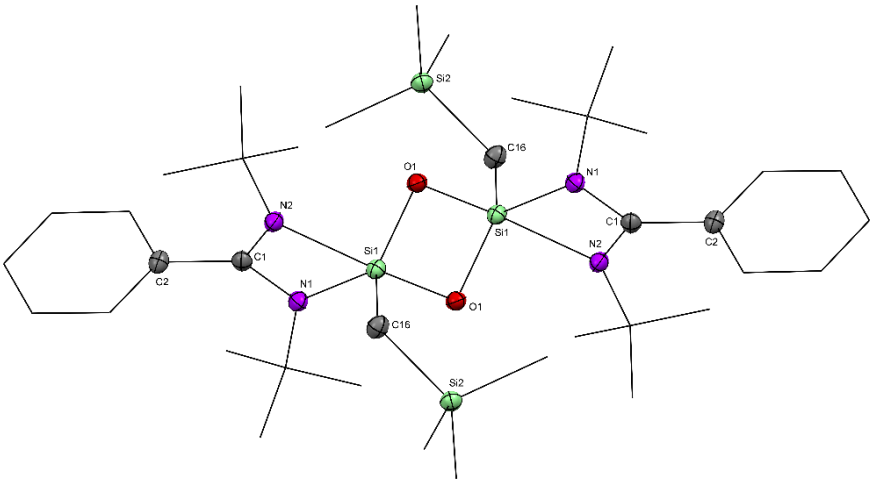


Figure S40. The molecular structure of **9**.

In spite of our several attempts, we were not able to prepare **9** in a reasonable scale. Though the molecular constitution of **9** is unequivocal, the data was not publishable and hence we refrain from discussing the structural parameters.

Crystal Data and Structure Refinement for 2-6.

X-ray Crystallography Details. The single-crystal structures of all the compounds were solved using X-ray intensity data recorded on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics with X-ray generator power setting at 50 kV and 1.4 mA. The intensity measurements were carried out with Mo (MoKα= 0.71073 Å) micro-focus sealed tube diffraction source. For all the compounds, the unit cell parameters were determined using 36 frames (matrix runs). The full intensity data were collected using an optimized strategy that consisted of different sets of ω, ϕ and 2θ with 0.5° width keeping the sample-to-detector distance fixed at 5.00 cm. The exposure time was set at 10-30 sec depending on the diffraction power of the crystals. The whole process of X-ray data acquisition was controlled and monitored by the APEX3[15] program suite. The complete data sets were corrected for Lorentz polarization and absorption effects using the APEX3 package through SAINT and SADABS programs. Using the APEX3 program suite, the structure was solved with the ShelXS-97[16] structure solution program, using direct methods. The model was refined with the version of ShelXL-2013[17] using Least Squares minimization. All the hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms. An ORTEP III[18] view of compounds **2-6** were drawn using the Mercury program[18] at the 50% probability displacement ellipsoids level and H atoms omitted for clarity.

Crystal data for compounds 2-4 and 6:

2. ($C_{25}H_{52}N_2Si_5$), red, 0.21 × 0.14 × 0.09 mm^3, monoclinic, space group '$P2_1/n$ ', a = 17.9412(7) Å, b = 10.1371(4) Å, c = 18.4496(8) Å, $\alpha = \gamma = 90$, β = 103.9940(10), V = 3255.9(2) Å^3, Z = 4, T = 100 (2) K, $2\theta_{max}$ = 74.84°, D_{calc} (g cm^{-3}) = 1.063, $F(000)$ = 1144, μ (mm^{-1}) = 0.235, 203335 reflections collected, 7850 unique reflections (R_{int} = 0.0721), 7074 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.6744, T_{max} = 0.7475, 304 refined parameters, S = 1.041, $R1$ = 0.0349, $wR2$ = 0.0997 (all data R = 0.0388, $wR2$ = 0.1028), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.868, $\Delta\rho_{min}$= -0.479 (eÅ^{-3}). CCDC: 2214132.

3. ($C_{19}H_{34}Cl_2N_2Si_2$), yellow, 0.21 × 0.15 × 0.08 mm^3, monoclinic, space group '$P2_1/n$', a = 6.2615(5) Å, b = 19.9686(14) Å, c = 18.2262(11) Å, $\alpha = \gamma = 90$, β = 98.455(2), V = 2254.1(3) Å^3, Z = 4, T = 196 (2) K, $2\theta_{max}$ = 56.56°, D_{calc} (g cm^{-3}) = 1.230, $F(000)$ = 896, μ (mm^{-1}) = 0.400, 124670 reflections collected, 5802 unique reflections (R_{int} = 0.0752), 4783 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.6823, T_{max} = 0.7457, 235 refined parameters, S = 1.079, $R1$ = 0.0327, $wR2$ = 0.0795 (all data R = 0.0454, $wR2$ = 0.0842), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.360, $\Delta\rho_{min}$= -0.391 (eÅ^{-3}). CCDC: 2214133.

4. ($C_{19}H_{34}N_2SSi_2$), yellow, 0.22 × 0.13 × 0.06 mm^3, monoclinic, space group '$C2/c$', a = 29.526(5) Å, b = 8.6554(15) Å, c = 17.895(3) Å, $\alpha = \gamma = 90$, β = 94.568(4), V = 4558.6(13) Å^3, Z = 8, T = 100 (2) K,

$2\theta_{max}$ = 56.81°, D_{calc} (g cm^{-3}) = 1.104, $F(000)$ = 1648, μ (mm^{-1}) = 0.251, 109201 reflections collected, 5716 unique reflections (R_{int} = 0.1790), 4170 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.4741, T_{max} = 0.7457, 231 refined parameters, S = 1.210, $R1$ = 0.0627, $wR2$ = 0.1755 (all data R = 0.0952, $wR2$ = 0.1937), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.712, $\Delta\rho_{min}$= -0.600 (eÅ^{-3}). CCDC: 2214134.

6. ($C_{25}H_{52}N_2Si_5Te$), red, 0.21 × 0.17 × 0.13 mm^3, orthorhombic, space group '$P21\ 21\ 21$', a = 14.873(3) Å, b = 19.141(3) Å, c = 12.115(2) Å, $\alpha = \beta = \gamma$ = 90, V = 3449.0(10) Å^3, Z = 4, T = 100 (2) K, $2\theta_{max}$ = 64.36°, D_{calc} (g cm^{-3}) = 1.249, $F(000)$ = 1352, μ (mm^{-1}) = 1.052, 93617 reflections collected, 8306 unique reflections (R_{int} = 0.1015), 7441 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.6002, T_{max} = 0.7470, 313 refined parameters, S = 1.108, $R1$ = 0.0548, $wR2$ = 0.1367 (all data R = 0.0659, $wR2$ = 0.1472), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 2.549, $\Delta\rho_{min}$= -1.134 (eÅ^{-3}). CCDC: 2214136.

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(II) PBE-D3/def2-TZVP optimized geometries of all structures discussed in the paper

(1) **1**
81

C	0.691850	15.193622	5.246979	H	4.020117	15.194298	6.222011	C	-0.255498	11.437350	10.899792
C	0.814529	15.926869	3.955919	H	4.435609	16.929159	6.283204	H	-0.654624	12.462271	10.883291
C	-0.019758	17.017760	3.666454	H	3.547562	16.273642	4.888325	H	0.661722	11.439689	11.504837
H	-0.751969	17.345419	4.405824	C	1.839554	17.909363	6.323019	H	-0.991811	10.791249	11.404451
C	0.096283	17.694486	2.451525	H	1.782819	18.051830	5.237607	C	0.842229	9.072425	9.258278
H	-0.557145	18.542906	2.241272	H	2.533872	18.661849	6.724778	H	0.203977	8.421291	9.877583
C	1.048324	17.290084	1.511327	H	0.845562	18.092511	6.756411	H	1.843675	9.095647	9.707135
H	1.137966	17.819042	0.560988	C	-1.270108	13.634628	4.732452	H	0.926906	8.610074	8.263829
C	1.886739	16.208951	1.794102	C	-0.775971	13.130162	3.366273	C	-1.662039	10.516500	8.381754
H	2.633575	15.888254	1.065919	H	-0.454868	13.955359	2.718205	H	-2.199748	9.785106	9.007127
C	1.772029	15.531609	3.009722	H	-1.590189	12.596480	2.855032	H	-1.609163	10.112952	7.361023
H	2.424148	14.683972	3.224902	H	0.068012	12.437785	3.489416	H	-2.255274	11.440601	8.356742
C	2.340183	16.502383	6.698845	C	-2.394033	14.671164	4.541523	C	2.665265	13.888602	10.916739
C	2.555593	16.460351	8.215094	H	-2.700968	15.082499	5.514129	H	1.871501	13.437860	11.529096
H	1.628034	16.715341	8.748380	H	-3.268256	14.194472	4.074188	H	2.285946	14.845661	10.537145
H	3.336275	17.174367	8.511138	H	-2.074719	15.496134	3.892702	H	3.523440	14.096732	11.576170
H	2.871034	15.459096	8.530001	C	-1.826596	12.459615	5.541192	C	3.730518	11.098305	10.429127
C	3.666282	16.204906	5.977696	H	-1.050198	11.707495	5.725288	H	4.576039	11.330749	11.096892
				H	-2.658093	11.982038	5.005054	H	4.057679	10.321571	9.724459
				H	-2.202542	12.810444	6.513145	H	2.921128	10.683768	11.045648

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H 3.480431 9.157344 7.498749
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Si 0.194653 14.320996 7.399445
Si 1.479223 12.290500 7.936491
Si 0.053380 10.796519 9.140408
Si 3.203469 12.693208 9.542557
Si 2.497967 11.060692 6.176711

(2) **$TMSCH_2Cl$**

17

Si 0.940963 -0.009697 -0.330840
C 0.086312 1.583718 0.205616
H -0.942532 1.636442 -0.180892
H 0.036436 1.640688 1.303642
H 0.631310 2.470099 -0.152480
C -0.045696 -1.513083 0.219010
H -1.065314 -1.487638 -0.193887
H 0.435402 -2.442190 -0.119314
H -0.124964 -1.548637 1.315895
C 2.701003 -0.075250 0.327948
H 2.703995 -0.125256 1.427242
H 3.229029 -0.960754 -0.054962
H 3.269660 0.817658 0.027701
C 0.996313 0.022397 -2.236518
H -0.010917 0.049935 -2.674826
H 1.559620 0.885638 -2.616871
Cl 1.807074 -1.457214 -2.906585

(3) **TS_1**

98

C 1.585376 15.645698 5.455028
C 2.150860 16.625778 4.490172
C 1.523246 17.863939 4.284192
H 0.616687 18.106856 4.841061
C 2.062024 18.784370 3.385383
H 1.567173 19.745259 3.235030
C 3.231357 18.477884 2.683456
H 3.651556 19.198807 1.980235
C 3.861490 17.247758 2.885150
H 4.774541 17.002487 2.340291
C 3.325042 16.325001 3.785257
H 3.816278 15.362597 3.938620
C 2.875497 16.259492 7.585156
C 2.561467 15.900979 9.041074
H 1.580806 16.295108 9.340801
H 3.321751 16.321157 9.712921
H 2.554208 14.812019 9.174158
C 4.296674 15.791388 7.226788
H 4.378774 14.700338 7.316631
H 5.029644 16.254756 7.902715
H 4.554820 16.073784 6.197693
C 2.773967 17.786900 7.426844
H 3.095761 18.124510 6.434785
H 3.423605 18.267348 8.172695
H 1.745253 18.133140 7.600368
C -0.174326 14.479138 3.997079
C 0.753732 14.026791 2.856750
H 1.413709 14.841352 2.532968
H 0.151667 13.713328 1.991683
H 1.377876 13.179481 3.168727
C -0.990324 15.701945 3.542152
H -1.623060 16.075008 4.358108
H -1.643594 15.413266 2.706136
H -0.343765 16.517455 3.197280
C -1.144339 13.351268 4.360137
H -0.600165 12.470342 4.723803
H -1.736713 13.056181 3.483964
H -1.838134 13.676623 5.148805
C -1.308281 10.850138 9.700639
H -1.606156 11.873083 9.975012
H -0.565600 10.511824 10.436155
H -2.195891 10.204488 9.802046
C -0.185934 8.889909 7.638641
H -1.038262 8.241840 7.899653
H 0.668734 8.590289 8.261048
H 0.074771 8.696789 6.588653
C -2.153361 11.058865 6.794686
H -2.979827 10.390345 7.085123
H -1.926004 10.875768 5.735760
H -2.510126 12.093851 6.895304
C 1.654670 12.801583 11.017787
H 0.581399 12.587632 11.112353
H 1.768628 13.891596 10.950174
H 2.147903 12.476128 11.948287
C 2.507128 10.045210 10.056203
H 3.119625 9.952615 10.967610
H 2.963524 9.421568 9.276168

H 1.510844 9.641681 10.279774
C 4.257657 12.425331 9.405458
H 4.365987 13.506341 9.249133
H 4.760713 11.910576 8.574460
H 4.792413 12.168140 10.334207
C 3.619679 9.651889 6.466832
H 2.979312 8.846035 6.853546
H 4.310422 9.953508 7.266333
H 4.219538 9.238442 5.639723
C 1.567541 10.409968 4.376754
H 2.251953 10.012624 3.609710
H 0.930066 11.163810 3.897363
H 0.919143 9.586317 4.707344
C 3.781305 12.407818 5.134084
H 4.378468 11.991562 4.307220
H 4.473674 12.758026 5.913276
H 3.229894 13.280385 4.757539
N 0.607832 14.744967 5.223384
N 1.891265 15.525625 6.763158
Si 0.453965 14.348817 7.059027
Si 1.236686 12.093930 7.509475
Si -0.673555 10.702194 7.923711
Si 2.446730 11.877260 9.565888
Si 2.587325 11.104573 5.818348
C -1.196746 14.768215 9.146508
H -1.666861 13.902492 8.684895
Si -1.874739 16.522990 8.877519
C -1.411994 17.290073 7.210438
H -0.324003 17.354965 7.072797
H -1.823197 16.698153 6.381263
H -1.829373 18.308429 7.145031
C -1.182407 17.646061 10.222791
H -1.415597 17.249535 11.219561
H -0.089371 17.745057 10.137615
H -1.614637 18.654329 10.132030
C -3.756245 16.447037 8.911300
H -4.126119 15.748466 8.144890
H -4.123960 16.108315 9.887940
H -4.178968 17.439859 8.692876
Cl -2.134082 14.409335 11.103884
H -0.208774 14.567808 9.556472

(4) **Int_1**

98

C -0.028226 0.123668 -2.300447
C -0.183343 0.456135 -3.741405
C 0.117410 -0.499693 -4.722498
H 0.457814 -1.493009 -4.428554
C -0.031291 -0.185577 -6.073822
H 0.200606 -0.937885 -6.829044
C -0.476285 1.082336 -6.455644
H -0.590433 1.326308 -7.512968
C -0.776469 2.036833 -5.480714
H -1.124048 3.029246 -5.771139
C -0.634622 1.726631 -4.127850
H -0.867497 2.476305 -3.371247
C -2.434975 -0.582633 -1.703272
C -2.956660 -1.176245 -0.392195
H -2.430239 -2.100422 -0.120713
H -4.026568 -1.406826 -0.478109
H -2.832364 -0.458600 0.427912
C -3.196872 0.714704 -2.019626
H -3.010514 1.475202 -1.249436
H -4.276518 0.510276 -2.048348
H -2.905073 1.125683 -2.994063
C -2.620355 -1.596025 -2.843553
H -2.336902 -1.174299 -3.815629
H -3.678586 -1.887165 -2.896810
H -2.026005 -2.502017 -2.666341
C 2.482225 0.582175 -1.959253
C 2.501998 1.984992 -2.588157
H 2.010013 1.995539 -3.568139
H 3.544091 2.303565 -2.730724
H 2.004226 2.719290 -1.942458
C 3.100549 -0.430697 -2.935845
H 3.089168 -1.440863 -2.508021
H 4.145903 -0.152380 -3.131924
H 2.570332 -0.445979 -3.895632
C 3.297499 0.573520 -0.662656
H 2.847649 1.229821 0.093416
H 4.320279 0.923260 -0.855634
H 3.361634 -0.441150 -0.246527
C 0.886849 -0.754479 4.585644
H 0.605556 -1.676767 4.047282
H -0.001151 -0.421907 5.141889
H 1.668102 -1.005333 5.322115
C 1.825689 2.175249 4.469490
H 2.494562 1.937597 5.312524
H 0.887894 2.567332 4.886035
H 2.300243 2.972452 3.880035
C 3.247638 0.051307 2.817481
H 3.887120 -0.147812 3.692626
H 3.739285 0.823474 2.210547
H 3.193506 -0.877068 2.232780
C -2.794373 -0.701492 3.212308
H -2.000021 -1.462265 3.299731
H -3.496967 -1.053100 2.444088
H -3.341700 -0.669872 4.168356
C -1.963067 1.948669 4.492484
H -2.954349 2.002760 4.971013
H -1.584942 2.972443 4.376573

H -1.294310 1.406269 5.173891
C -3.494265 1.999718 1.871530
H -3.734345 1.537790 0.904651
H -3.196299 3.041337 1.687679
H -4.420857 2.014692 2.468127
C -0.477461 4.595246 2.310651
H 0.022502 4.490165 3.283890
H -1.555918 4.452437 2.460641
H -0.318262 5.627921 1.960514
C 2.061859 3.922670 0.832930
H 2.096510 4.997570 0.592451
H 2.590428 3.385065 0.036869
H 2.620349 3.772013 1.767801
C -0.653053 3.692053 -0.613889
H -0.537530 4.737704 -0.940052
H -1.727460 3.479426 -0.519547
H -0.245654 3.044179 -1.401337
N 1.104199 0.184806 -1.573916
N -0.998137 -0.298654 -1.465828
Si 0.195101 -0.399593 -0.060862
Si -0.035997 1.145368 1.734655
Si 1.551202 0.592957 3.457861
Si -2.174800 1.039627 2.841737
Si 0.248019 3.406562 1.027720
C 0.690726 -2.094609 0.458608
H 1.746491 -1.968646 0.767030
Si 0.595787 -3.758564 -0.469825
C 1.089714 -3.627481 -2.292484
H 0.444259 -2.920492 -2.833358
H 2.134329 -3.314561 -2.426214
H 0.973937 -4.612005 -2.772004
C -1.127708 -4.505036 -0.374717
H -1.485575 -4.438831 0.665481
H -1.855169 -4.029161 -1.046822
H -1.068102 -5.568873 -0.653617
C 1.802996 -4.883752 0.432388
H 2.833726 -4.500767 0.382954
H 1.495522 -4.937126 1.488485
H 1.792811 -5.899837 0.009670
Cl -0.672966 -3.664921 3.122867
H 0.160891 -2.332811 1.418771

(5) **TS_2**

98

C 0.071072 15.926503 5.572276
C 0.087703 16.788460 4.361039
C -0.985316 17.649075 4.088243
H -1.833591 17.696399 4.771482
C -0.956416 18.467195 2.958894
H -1.793705 19.137029 2.758001
C 0.139432 18.430881 2.092883
H 0.159443 19.070301 1.209094
C 1.210413 17.575171 2.362125
H 2.068374 17.538969 1.689411
C 1.188931 16.758193 3.493065
H 2.022113 16.084165 3.693226
C 1.509904 17.344000 7.159067
C 1.572757 17.292892 8.689234
H 0.579835 17.456002 9.132168
H 2.246395 18.074654 9.063379
H 1.958998 16.325235 9.034614
C 2.925844 17.230625 6.571806
H 3.379440 16.264872 6.826314
H 3.563933 18.030341 6.974203
H 2.907614 17.328921 5.478962
C 0.877112 18.681063 6.741490
H 0.927832 18.848515 5.659865
H 1.427610 19.495761 7.232617
H -0.173261 18.739747 7.057862
C -1.323434 13.948176 4.710861
C -0.505014 13.696672 3.434774
H -0.318339 14.622011 2.876546
H -1.064248 13.015661 2.778266
H 0.458941 13.226555 3.668705
C -2.641202 14.656011 4.354443
H -3.220422 14.893400 5.256714
H -3.249673 13.991851 3.724850
H -2.466368 15.582316 3.793283
C -1.636901 12.613083 5.383502
H -0.716926 12.098506 5.688574
H -2.183105 11.957619 4.692631
H -2.260336 12.753649 6.275845
C 1.744448 9.535068 8.680856
H 1.880458 8.890106 9.557460
H 2.697460 10.009088 8.409664
H 1.420352 8.889689 7.851904
C -1.269728 10.656889 8.123595
H -1.885837 9.911499 8.642236
H -1.123328 10.332504 7.084173
H -1.789134 11.625681 8.117420
C 0.155385 11.430697 10.811315
H -0.596448 10.801438 11.305088
H -0.161665 12.483347 10.827755
H 1.091604 11.343562 11.379483
C 2.322886 14.349097 11.095065
H 1.672767 13.655734 11.643555
H 1.724919 15.231994 10.831527
H 3.121562 14.680273 11.778174
C 4.012644 11.955218 10.260557
H 4.700471 12.264171 11.064286
H 4.605823 11.460799 9.479342

H	3.315201	11.215647	10.674686
C	4.487917	14.649142	8.951668
H	4.135565	15.677596	8.801466
H	4.917892	14.293934	8.004878
H	5.299303	14.683995	9.696873
C	4.549486	11.414055	6.519422
H	4.444906	10.485755	7.097983
H	5.158294	12.116741	7.104910
H	5.104644	11.172432	5.598426
C	1.982395	10.837697	4.993552
H	2.612922	10.556609	4.134786
H	1.016489	11.184750	4.602814
H	1.795892	9.932374	5.588673
C	3.233504	13.654168	4.940655
H	3.767132	13.341087	4.029146
H	3.859284	14.387349	5.468764
H	2.306890	14.157249	4.633906
N	-0.552231	14.737892	5.709859
N	0.693432	16.177352	6.737639
Si	0.146889	14.534835	7.425151
Si	1.567793	12.729829	7.945937
Si	0.367284	10.782988	9.049077
Si	3.126552	13.495360	9.603252
Si	2.870130	12.147208	6.035031
C	-1.059212	14.803367	8.830479
H	-1.194846	13.806300	9.285255
H	-0.457853	15.360547	9.572571
Cl	-0.677376	8.315159	10.304610
Si	-2.781397	15.603812	8.786077
C	-2.837075	17.103323	7.644619
H	-2.629375	16.818333	6.604405
H	-3.834774	17.566672	7.673423
H	-2.103886	17.864810	7.947315
C	-3.169622	16.156578	10.545003
H	-4.182082	16.583301	10.609445
H	-3.114720	15.309190	11.244871
H	-2.457380	16.923293	10.886410
C	-4.048903	14.319413	8.246788
H	-3.896547	13.979669	7.212626
H	-4.006198	13.433742	8.898677
H	-5.065361	14.736022	8.311862

(6) **2**

84

C	11.503374	5.026917	9.175443
C	12.344259	6.227584	9.432358
C	12.482949	7.204581	8.435760
H	11.988846	7.071451	7.472534
C	13.251839	8.344609	8.673406
H	13.354560	9.097395	7.890165
C	13.884675	8.520824	9.906351
H	14.483414	9.414000	10.091691
C	13.745984	7.550995	10.902675
H	14.234054	7.683221	11.869542
C	12.979838	6.408937	10.668498
H	12.860982	5.663087	11.454916
C	9.139315	5.940435	9.669608
C	7.920136	5.145210	10.164416
H	7.573789	4.447033	9.387292
H	7.097377	5.834152	10.399215
H	8.164894	4.575706	11.072777
C	8.753652	6.730699	8.406891
H	9.607800	7.312657	8.034238
H	7.935233	7.428716	8.634445
H	8.420427	6.042224	7.616576
C	9.595375	6.900540	10.778577
H	9.962634	6.350385	11.656389
H	8.734242	7.507685	11.090888
H	10.382922	7.585344	10.441960
C	13.263708	3.337215	8.349614
C	13.888483	4.165549	7.214310
H	13.239745	4.165677	6.328863
H	14.857133	3.730654	6.929083
H	14.062409	5.204831	7.522406
C	14.195923	3.346190	9.572975
H	14.428652	4.368809	9.895694
H	15.143015	2.849234	9.317453
H	13.743158	2.806941	10.416010
C	13.065889	1.892269	7.871850
H	12.664430	1.259970	8.676565
H	14.025555	1.466427	7.550030
H	12.366590	1.853071	7.025226
C	10.344153	-0.288918	6.428275
H	10.779962	-0.268312	7.438207
H	11.104664	0.086518	5.728264
H	10.134276	-1.341005	6.173198
C	7.501472	-0.077075	7.510708
H	7.375672	-1.143219	7.260238
H	6.519584	0.413305	7.436535
H	7.828138	-0.011812	8.558609
C	8.057920	0.471004	4.569075
H	7.871244	-0.601061	4.393955
H	8.762021	0.820562	3.799729
H	7.109733	1.010816	4.428193
C	8.753218	4.203222	3.445763
H	7.953482	4.890196	3.759944
H	8.281716	3.254029	3.151439
H	9.247107	4.629385	2.557374
C	10.748597	5.655682	5.228054
H	11.519548	5.583211	6.007462
H	9.975654	6.356409	5.574170

H 11.218642 6.078594 4.325716
C 11.402889 2.878007 4.124315
H 11.849258 3.377437 3.248344
H 11.017950 1.901430 3.795682
H 12.203329 2.689565 4.853536
C 9.742656 1.946194 9.873263
H 9.881875 0.971320 9.372810
C 9.080469 1.091695 12.721267
H 9.441720 0.909469 13.744817
H 8.682570 0.144438 12.327222
H 8.245788 1.807174 12.779674
C 11.868458 0.497765 11.586020
H 12.716550 0.836630 10.974047
H 11.522926 -0.464101 11.177430
H 12.243942 0.315774 12.604631
C 11.097758 3.364350 12.366536
H 10.323293 4.143909 12.379670
H 11.958336 3.745520 11.801080
H 11.423532 3.190755 13.403308
N 10.171853 4.936329 9.327911
N 11.916658 3.834583 8.702704
Si 10.141090 3.236436 8.555183
Si 8.815484 3.077474 6.698392
Si 8.744680 0.740082 6.323742
Si 10.004018 3.945206 4.854662
Si 10.460134 1.755783 11.615911
H 8.646892 2.040980 9.981054

(7) **TMSCl**

14

Si -0.740857 0.000069 -1.456349
C -1.680015 1.549046 -0.979924
H -2.679264 1.559073 -1.437869
H -1.801639 1.593000 0.113690
H -1.142397 2.451894 -1.302932
C -1.679187 -1.549656 -0.980732
H -2.675160 -1.563813 -1.445648
H -1.137082 -2.452310 -1.296721
H -1.808417 -1.589996 0.112143
C 0.998766 0.000511 -0.761582
H 0.964145 -0.000128 0.339136
H 1.553700 -0.890400 -1.088526
H 1.552981 0.892252 -1.087492
Cl -0.568393 0.000460 -3.556553

(8) **TS_1'**

98

C 0.912665 15.665882 5.859985
C 1.377591 16.980173 5.345609
C 1.228430 18.146153 6.112840
H 0.781068 18.082943 7.105582
C 1.675370 19.373635 5.623499
H 1.559716 20.271977 6.232008
C 2.273477 19.451188 4.362482
H 2.621423 20.412320 3.980446
C 2.425770 18.294722 3.593339
H 2.888830 18.348257 2.606751
C 1.982153 17.064949 4.082275
H 2.088317 16.165037 3.474535
C 3.107630 14.729887 6.792302
C 3.320558 13.564011 7.762962
H 2.748961 13.714670 8.689301
H 4.383716 13.470104 8.022087
H 2.995187 12.621296 7.307837
C 3.979444 14.519955 5.542339
H 3.682359 13.605655 5.011177
H 5.036999 14.429861 5.829728
H 3.886020 15.366216 4.849779
C 3.514714 16.034670 7.499876
H 3.519954 16.893489 6.818578
H 4.530117 15.922402 7.906770
H 2.835799 16.256952 8.335444
C -1.606510 15.828582 5.416179
C -1.442937 16.307505 3.963898
H -0.771212 17.171170 3.884744
H -2.424735 16.607852 3.571392
H -1.050100 15.502404 3.326862
C -2.048451 16.997104 6.315304
H -2.161876 16.654582 7.352320
H -3.021290 17.376170 5.970220
H -1.333163 17.828675 6.282229
C -2.678968 14.739891 5.479855
H -2.388432 13.867310 4.882473
H -3.632339 15.124168 5.092257
H -2.831442 14.420970 6.519013
C -1.965811 9.946894 8.221614
H -1.751746 10.779981 8.907227
H -1.159866 9.205197 8.310775
H -2.904617 9.470805 8.546966
C -2.498753 9.148269 5.272095
H -3.392562 8.603566 5.617769
H -1.666822 8.435025 5.213248
H -2.704722 9.514324 4.255282
C -3.728546 11.652676 6.429314
H -4.576916 10.999639 6.691937
H -3.929619 12.087841 5.440939
H -3.677467 12.462995 7.169212
C 1.931007 10.089743 8.241879
H 1.014626 9.922473 8.824389
H 2.391026 11.015825 8.607895
H 2.626003 9.260833 8.452501
C 1.040213 8.352269 5.933774
H 1.888337 7.677126 6.133273

H 0.767643 8.251100 4.874626
H 0.191083 8.012087 6.542796
C 3.185606 10.431371 5.442285
H 3.615602 11.422514 5.637690
H 3.038868 10.339463 4.356523
H 3.929742 9.677638 5.746217
C 0.354790 10.146664 2.609551
H -0.403159 9.390994 2.860601
H 1.333626 9.767964 2.933638
H 0.378314 10.252378 1.512627
C -1.714450 12.355420 2.616296
H -1.642668 12.255599 1.521118
H -1.971943 13.398243 2.841408
H -2.543930 11.719802 2.958263
C 1.263270 13.075424 2.872893
H 1.287048 13.189605 1.777659
H 2.260615 12.757069 3.207982
H 1.057264 14.058614 3.319533
N -0.355080 15.209960 5.913848
N 1.677366 14.695054 6.416082
Si 0.146427 13.756508 7.000716
Si -0.143493 11.680887 5.764950
Si -2.162927 10.596228 6.454567
Si 1.564429 10.119818 6.382079
Si -0.064610 11.826445 3.388011
Cl -2.384543 14.101088 9.117796
C -0.377284 15.391344 9.326802
H 0.339730 15.666634 8.548566
H -1.128924 16.175483 9.444097
Si 0.237108 14.607763 10.925093
C 1.899738 15.435360 11.317325
H 1.803931 16.530378 11.365315
H 2.268261 15.085351 12.294376
H 2.665248 15.193911 10.565434
C 0.483680 12.749864 10.794684
H 0.842442 12.337725 11.750082
H -0.470503 12.271437 10.534312
H 1.210915 12.494702 10.012534
C -0.987097 15.012910 12.296163
H -1.104771 16.100338 12.417172
H -1.971739 14.583617 12.064222
H -0.641550 14.600552 13.256402

(9) **Int_1'**

98

C -0.203950 0.254385 -2.093672
C -0.684236 0.535647 -3.479544
C 0.244936 0.595045 -4.528329
H 1.306063 0.463616 -4.316380
C -0.183307 0.807802 -5.838379
H 0.549306 0.843423 -6.646414
C -1.543036 0.977035 -6.114313
H -1.877938 1.146359 -7.138949
C -2.471134 0.933293 -5.070716
H -3.533655 1.076043 -5.274974
C -2.045183 0.709942 -3.760710
H -2.772583 0.695645 -2.949151
C -0.840126 -2.182023 -2.007372
C -0.249983 -3.348558 -1.199464
H 0.795786 -3.538334 -1.476536
H -0.819367 -4.264384 -1.410748
H -0.300668 -3.156969 -0.122584
C -2.368299 -2.187394 -1.815358
H -2.627689 -1.992973 -0.767070
H -2.781075 -3.166864 -2.098822
H -2.847838 -1.425198 -2.441188
C -0.512909 -2.466825 -3.487531
H -1.071321 -1.832494 -4.183549
H -0.776193 -3.512453 -3.704480
H 0.561055 -2.342939 -3.684191
C 0.581174 2.638698 -1.469945
C -0.314978 3.240007 -2.568699
H -0.017970 2.956290 -3.583178
H -0.223396 4.332627 -2.488854
H -1.373635 2.986089 -2.427122
C 2.040341 2.988151 -1.811013
H 2.730258 2.604190 -1.051428
H 2.158965 4.079901 -1.871702
H 2.312503 2.563007 -2.788311
C 0.128999 3.317417 -0.163859
H -0.944634 3.145344 -0.010020
H 0.290411 4.402287 -0.241445
H 0.675080 2.952474 0.708968
C 1.707153 0.125797 4.561092
H 2.503145 0.112583 3.803855
H 1.482247 -0.911523 4.848871
H 2.083801 0.650667 5.453471
C -1.138665 1.000420 5.277854
H -0.787457 1.672826 6.077519
H -1.292186 0.007873 5.716906
H -2.115148 1.373332 4.938988
C 0.581979 2.846439 3.659947
H 0.841829 3.259385 4.648544
H -0.275876 3.413360 3.274364
H 1.432340 2.994883 2.984868
C 0.629654 -3.338989 2.671566
H 1.432429 -2.787292 3.181969
H 0.970765 -3.550404 1.650254
H 0.492745 -4.300701 3.191716
C -1.527253 -2.404601 4.557988
H -1.735203 -3.453771 4.824934

H -2.439925 -1.822443 4.745141
H -0.737179 -2.039315 5.227334
C -2.350038 -3.385315 1.865672
H -2.219728 -3.488405 0.783408
H -3.342601 -2.950077 2.048869
H -2.345503 -4.397118 2.302927
C -4.172018 -0.023542 2.532760
H -3.918947 -0.153788 3.594762
H -4.342856 -1.018566 2.098933
H -5.118628 0.537766 2.476881
C -2.875254 2.704315 2.268067
H -3.879681 3.113242 2.069901
H -2.142282 3.360517 1.780636
H -2.703167 2.752570 3.351673
C -3.342160 1.048371 -0.212981
H -4.289800 1.605764 -0.279511
H -3.489588 0.060539 -0.665903
H -2.587612 1.588144 -0.801024
N 0.459138 1.148074 -1.304389
N -0.279508 -0.908478 -1.476448
Si 0.868620 -0.031460 0.089056
Si -0.689811 -0.115115 1.946998
Si 0.170601 1.011086 3.893714
Si -1.000749 -2.369662 2.735245
Si -2.820178 0.927276 1.602755
Cl 2.392520 1.299909 1.130996
C 2.183400 -1.387466 -0.000519
H 2.590309 -1.438963 1.023434
H 1.692353 -2.346177 -0.196101
Si 3.711742 -1.345212 -1.122896
C 4.309415 -3.136178 -1.255167
H 3.546066 -3.777214 -1.723095
H 5.224961 -3.203790 -1.862480
H 4.531065 -3.551108 -0.260101
C 5.104899 -0.298945 -0.406980
H 6.016890 -0.422071 -1.011930
H 4.835847 0.765641 -0.388586
H 5.334679 -0.600370 0.625752
C 3.324311 -0.723901 -2.861392
H 2.528031 -1.318047 -3.332489
H 3.003609 0.326523 -2.830206
H 4.218438 -0.789470 -3.499645

(10) **TS_2'**

98

C 0.326134 15.627441 5.262663
C 0.329291 16.394722 3.989579
C -0.622776 17.400864 3.775648
H -1.374048 17.606673 4.538953
C -0.598889 18.145991 2.597335
H -1.340855 18.930241 2.439862
C 0.370493 17.888809 1.623335
H 0.386656 18.471375 0.700875
C 1.317780 16.883253 1.832886
H 2.073473 16.673778 1.074299
C 1.301673 16.138828 3.013843
H 2.034781 15.346993 3.172720
C 2.168980 16.911608 6.514464
C 2.356915 17.057106 8.030333
H 1.458296 17.479606 8.500774
H 3.201615 17.727098 8.239104
H 2.574595 16.087020 8.494996
C 3.486758 16.447640 5.871145
H 3.778628 15.461764 6.253258
H 4.291044 17.161361 6.101212
H 3.388206 16.385650 4.779539
C 1.775343 18.287791 5.951459
H 1.776270 18.312338 4.856289
H 2.508076 19.027504 6.304209
H 0.783391 18.595378 6.309259
C -1.458150 13.800992 4.810432
C -1.601082 14.245688 3.349053
H -1.992715 15.264620 3.249543
H -2.317582 13.562914 2.871459
H -0.654835 14.176686 2.797829
C -2.816659 13.955123 5.510225
H -2.757142 13.614471 6.550607
H -3.571629 13.343998 4.995386
H -3.150555 15.002170 5.489517
C -1.024062 12.328992 4.813101
H -0.096551 12.203916 4.240091
H -1.804137 11.712924 4.343511
H -0.873183 11.959382 5.835044
C 0.204936 11.340249 10.910483
H -0.272813 12.326091 10.988042
H 1.267710 11.451355 11.161386
H -0.259695 10.677624 11.657835
C 1.397733 9.387210 8.751112
H 1.425242 8.605430 9.530501
H 2.387309 9.854910 8.679783
H 1.183588 8.886606 7.795195
C -1.363046 9.216174 9.390193
H -0.948860 8.392473 9.995326
H -1.652494 8.801031 8.412480
H -2.274176 9.593121 9.873329
C 2.694800 14.190568 10.748440
H 1.847271 13.709752 11.254602
H 2.376874 15.198918 10.449001
H 3.511052 14.306073 11.480306
C 4.094583 11.583976 10.045787
H 4.876640 11.890286 10.759386

H 4.567118 10.954113 9.279115
H 3.363748 10.968193 10.586392
C 4.799389 14.096093 8.547797
H 4.570731 15.152736 8.359666
H 5.149912 13.653780 7.605412
H 5.633712 14.060819 9.267669
C 4.423905 10.925719 6.270939
H 4.384970 10.136549 7.036187
H 5.108968 11.708983 6.622308
H 4.854091 10.482281 5.358124
C 1.771384 10.076866 5.147413
H 2.104817 9.906505 4.110894
H 0.680162 10.188637 5.143420
H 2.013812 9.176052 5.728952
C 2.885661 12.853034 4.476595
H 3.372748 12.385590 3.605657
H 3.501038 13.703976 4.799829
H 1.910353 13.241517 4.151290
N -0.449049 14.574817 5.590882
N 1.123424 15.878260 6.316001
Si 0.419008 14.417012 7.248350
Si 1.568132 12.443937 7.807828
Si -0.037571 10.592256 9.185532
Si 3.320428 13.146567 9.285814
Si 2.684394 11.580112 5.874999
Cl -1.743404 11.894711 8.287060
C -0.473494 15.106884 8.746170
H -0.759930 14.214947 9.327748
H 0.349723 15.576169 9.313437
Si -1.943380 16.301547 8.846974
C -1.670529 17.372352 10.379936
H -0.755905 17.977871 10.284884
H -2.515521 18.059369 10.540000
H -1.566980 16.747756 11.280208
C -3.543879 15.332763 9.060849
H -4.383278 16.019140 9.250830
H -3.787022 14.732712 8.173972
H -3.465815 14.642290 9.913704
C -2.091150 17.441740 7.349899
H -1.174471 18.027662 7.191591
H -2.295184 16.864306 6.437777
H -2.922283 18.148415 7.494885

(11) **Ph_3PS**

35

P -0.438513 0.192764 -0.246323
S 1.346471 -0.406547 -0.807384
C -0.814850 -0.162353 1.511401
C -0.356862 -1.370208 2.058475
C -1.557603 0.722859 2.306085
C -0.649356 -1.692560 3.383745
C -1.843145 0.397885 3.635080
C -1.392790 -0.809509 4.173798
H 0.242726 -2.043912 1.442678
H -1.907049 1.670642 1.893403
H -0.289013 -2.633251 3.803695
H -2.414772 1.094660 4.250731
H -1.614037 -1.060271 5.212792
C -0.698850 1.997533 -0.428012
C 0.374164 2.853971 -0.139019
C -1.932136 2.537282 -0.820914
C 0.209315 4.236074 -0.229962
C -2.089934 3.922500 -0.917827
C -1.022571 4.772389 -0.619108
H 1.339675 2.427392 0.140575
H -2.769031 1.879279 -1.059443
H 1.047856 4.896848 -0.003372
H -3.049971 4.336058 -1.231673
H -1.147548 5.853994 -0.696341
C -1.806172 -0.585519 -1.185018
C -1.597686 -0.894601 -2.536762
C -3.049330 -0.855327 -0.593965
C -2.627262 -1.456700 -3.292041
C -4.075403 -1.423430 -1.353166
C -3.867126 -1.721264 -2.701923
H -0.619005 -0.706151 -2.983320
H -3.216854 -0.631507 0.460937
H -2.458255 -1.695600 -4.343518
H -5.038166 -1.637847 -0.885837
H -4.669149 -2.167594 -3.292590

(12) **Ph_3PSe**

35

P -0.435388 0.191939 -0.247748
C -0.808003 -0.164797 1.510431
C -0.352833 -1.372957 2.058518
C -1.551726 0.722372 2.302480
C -0.648278 -1.694257 3.383092
C -1.840225 0.397806 3.630963
C -1.391922 -0.809638 4.171274
H 0.247462 -2.047709 1.444387
H -1.901443 1.669475 1.888531
H -0.290149 -2.635555 3.803683
H -2.414169 1.094924 4.244305
H -1.614478 -1.058465 5.210309
C -0.692602 1.996902 -0.430125
C 0.378573 2.854764 -0.139608
C -1.927445 2.533656 -0.822959
C 0.211118 4.236294 -0.229338
C -2.087517 3.918760 -0.918157
C -1.021716 4.770377 -0.618731
H 1.344991 2.429715 0.139660
H -2.763747 1.874624 -1.060579

H 1.048488 4.898226 -0.001499
H -3.049178 4.330445 -1.229874
H -1.148753 5.851559 -0.696435
C -1.800886 -0.588337 -1.187922
C -1.595124 -0.896257 -2.540123
C -3.043137 -0.856710 -0.593762
C -2.626350 -1.456657 -3.293754
C -4.071007 -1.422841 -1.352063
C -3.865302 -1.720409 -2.701321
H -0.616816 -0.708909 -2.988424
H -3.209616 -0.631697 0.461049
H -2.459044 -1.694716 -4.345766
H -5.033860 -1.634334 -0.883294
H -4.668627 -2.166473 -3.290132
Se 1.495117 -0.454850 -0.856815

(13) **Ph_3PTe**

35

P -0.414753 0.185065 -0.249523
C -0.792367 -0.166247 1.509383
C -0.411533 -1.405408 2.045757
C -1.472300 0.760785 2.312689
C -0.718477 -1.717011 3.369622
C -1.768090 0.446655 3.642255
C -1.395498 -0.790990 4.170694
H 0.141631 -2.113184 1.424156
H -1.766704 1.729405 1.906536
H -0.419071 -2.682754 3.780192
H -2.288531 1.175919 4.265529
H -1.625930 -1.033198 5.209652
C -0.678717 1.989290 -0.438087
C 0.360226 2.862799 -0.083016
C -1.897335 2.508086 -0.899473
C 0.176040 4.241657 -0.177702
C -2.072049 3.890908 -1.002668
C -1.039337 4.758025 -0.639711
H 1.316684 2.453513 0.250027
H -2.708814 1.836968 -1.183747
H 0.987896 4.915413 0.101562
H -3.019496 4.288474 -1.370686
H -1.177787 5.837476 -0.722869
C -1.781681 -0.597077 -1.188161
C -1.617299 -0.833438 -2.560735
C -2.993427 -0.929723 -0.564545
C -2.659853 -1.387113 -3.303453
C -4.030960 -1.492730 -1.312095
C -3.867379 -1.719024 -2.680417
H -0.662459 -0.596665 -3.036354
H -3.128395 -0.755421 0.503891
H -2.525429 -1.568028 -4.371298
H -4.968528 -1.756773 -0.819647
H -4.678527 -2.161223 -3.261623
Te 1.739642 -0.533688 -0.915587

(14) **Zwitter ion of S**

85

C 11.112516 3.748897 8.104591
C 11.375432 5.206501 8.196286
C 11.730437 5.921682 7.042673
H 11.796935 5.405626 6.084563
C 11.986428 7.290449 7.119325
H 12.255277 7.839602 6.215803
C 11.902997 7.952530 8.347268
H 12.109697 9.022263 8.406830
C 11.559008 7.240991 9.499494
H 11.502094 7.750487 10.462702
C 11.290849 5.873672 9.425857
H 11.044273 5.317750 10.330929
C 8.532949 3.697158 8.137669
C 7.607830 2.503102 7.869566
H 7.833938 2.039817 6.898748
H 6.559686 2.829801 7.855348
H 7.713299 1.736801 8.651906
C 8.351748 4.738048 7.021688
H 8.956664 5.636283 7.198021
H 7.297334 5.044435 6.974861
H 8.628993 4.316431 6.046390
C 8.179605 4.319200 9.498942
H 8.353020 3.604086 10.314673
H 7.117928 4.604249 9.511445
H 8.772802 5.221601 9.691946
C 13.509850 2.803305 7.872657
C 13.981204 2.981009 6.420630
H 13.578259 2.171424 5.792867
H 15.079525 2.940180 6.379076
H 13.659660 3.952948 6.021558
C 14.090032 3.908904 8.767187
H 13.914731 4.914718 8.368470
H 15.176740 3.760721 8.831043
H 13.679981 3.858261 9.785510
C 13.987291 1.440355 8.398914
H 13.675284 1.287238 9.442174
H 15.084668 1.400965 8.360631
H 13.593847 0.625869 7.770654
C 8.793448 -1.996627 3.996874
H 9.810873 -2.254428 3.668351
H 8.363708 -1.297614 3.264287
H 8.184041 -2.914159 3.990646
C 9.405382 -2.593836 6.939018
H 8.888960 -3.542553 6.723144
H 9.200558 -2.330669 7.987093
H 10.489093 -2.748357 6.829046
C 7.064222 -0.725018 6.197092

H	6.385576	-1.586498	6.089593
H	6.692872	0.079587	5.545421
H	6.999890	-0.376157	7.238064
C	8.171477	2.262268	3.581017
H	7.731308	2.754294	4.460600
H	7.619328	1.326027	3.411458
H	8.002568	2.916058	2.710508
C	10.931352	3.581308	3.957483
H	12.004981	3.423435	4.131242
H	10.531277	4.175311	4.791085
H	10.811990	4.171085	3.035092
C	10.678145	1.041860	2.258864
H	10.617211	1.700909	1.378395
H	10.103656	0.128454	2.046383
H	11.727054	0.748029	2.411034
C	10.692817	0.278825	9.123265
H	11.597272	-0.323466	8.927764
C	8.779019	0.642923	11.494655
H	8.678283	0.822984	12.575736
H	8.325620	-0.335485	11.273263
H	8.188542	1.410221	10.972910
C	11.526826	-0.681631	11.896101
H	12.592576	-0.678192	11.620724
H	11.121971	-1.675586	11.652998
H	11.457141	-0.542130	12.985652
C	11.335294	2.344012	11.439207
H	10.784844	3.165883	10.961276
H	12.391413	2.422661	11.145727
H	11.277438	2.486360	12.529103
N	9.905909	3.141191	8.160927
N	12.022003	2.777869	7.898954
Si	10.689450	1.513243	7.717526
Si	10.485529	0.469834	5.623088
Si	8.832483	-1.245713	5.738392
Si	10.027398	1.921224	3.801887
Si	10.593417	0.672874	10.974275
H	9.858462	-0.409542	8.902008
S	12.381747	-0.399405	5.585560

(15) **Zwitter ion of Se 85**

C	11.122822	3.737967	8.095486
C	11.366664	5.198354	8.191836
C	11.719804	5.919457	7.041364
H	11.800577	5.404925	6.083624
C	11.956603	7.291403	7.120988
H	12.224215	7.845042	6.219856
C	11.856370	7.950854	8.349097
H	12.048461	9.023141	8.411254
C	11.514978	7.233412	9.498408
H	11.445796	7.740910	10.461867
C	11.265462	5.862780	9.421557
H	11.021494	5.302454	10.324538
C	8.545518	3.655307	8.138940
C	7.634014	2.452753	7.863525
H	7.860984	2.001706	6.887426
H	6.581822	2.766652	7.857834
H	7.752993	1.680000	8.637615
C	8.352365	4.699989	7.028622
H	8.940781	5.607458	7.213109
H	7.293067	4.988502	6.979015
H	8.640770	4.289285	6.051969
C	8.183400	4.266433	9.502740
H	8.363820	3.549651	10.315342
H	7.118447	4.538980	9.514565
H	8.765554	5.174946	9.700545
C	13.533348	2.827644	7.864735
C	14.015198	2.994446	6.415128
H	13.625479	2.175655	5.791074
H	15.113999	2.962210	6.382702
H	13.688701	3.959332	6.003079
C	14.091325	3.952510	8.749592
H	13.910157	4.950900	8.335412
H	15.178773	3.816295	8.826119
H	13.672172	3.911437	9.764619
C	14.029068	1.480819	8.414612
H	13.715719	1.339765	9.459111
H	15.127015	1.458245	8.380382
H	13.651543	0.649071	7.799506
C	8.791271	-2.013256	4.018165
H	9.821431	-2.288793	3.749029
H	8.406735	-1.328644	3.247782
H	8.171810	-2.923928	4.005297
C	9.223421	-2.533572	7.013638
H	8.693620	-3.475223	6.799107
H	8.961533	-2.229052	8.037692
H	10.306414	-2.721444	6.972427
C	6.967911	-0.655987	6.086273
H	6.283589	-1.508616	5.947722
H	6.647963	0.146396	5.405580
H	6.848073	-0.295424	7.118014
C	8.187284	2.289681	3.547510
H	7.735338	2.773341	4.425723
H	7.628716	1.362389	3.352029
H	8.043878	2.957961	2.683407
C	10.959991	3.565654	3.976295
H	12.026980	3.391234	4.172488
H	10.550202	4.163797	4.802066
H	10.868944	4.158456	3.052725
C	10.692893	1.033439	2.264151
H	10.646716	1.693265	1.383362

H 10.111580 0.125712 2.046282
H 11.737026 0.729014 2.427898
C 10.765636 0.265317 9.120599
H 11.690053 -0.307718 8.932783
C 8.831096 0.597451 11.482014
H 8.720594 0.785116 12.560884
H 8.401396 -0.393129 11.267456
H 8.225910 1.346199 10.950177
C 11.602980 -0.671171 11.898153
H 12.668665 -0.650296 11.623355
H 11.215282 -1.672689 11.658223
H 11.530292 -0.528813 12.987158
C 11.353087 2.349569 11.435485
H 10.786239 3.159444 10.956340
H 12.408186 2.450655 11.145027
H 11.289177 2.490641 12.525216
N 9.925517 3.115059 8.160914
N 12.044598 2.780725 7.876076
Si 10.728060 1.495130 7.712825
Si 10.431968 0.468579 5.629698
Si 8.748707 -1.217395 5.738334
Si 10.033845 1.921746 3.796604
Si 10.646876 0.662914 10.969863
H 9.956780 -0.452021 8.897565
Se 12.432950 -0.539147 5.572367

(16) **Zwitter ion of Te 85**

C 11.137599 3.729083 8.081140
C 11.363944 5.191946 8.182160
C 11.715445 5.919407 7.035179
H 11.811484 5.407750 6.077349
C 11.931301 7.294540 7.118169
H 12.196936 7.853090 6.219512
C 11.812574 7.950888 8.346325
H 11.987017 9.026045 8.410795
C 11.475382 7.226698 9.492636
H 11.393145 7.731423 10.456516
C 11.246351 5.852755 9.412285
H 11.006315 5.287386 10.313084
C 8.562096 3.623952 8.120475
C 7.660668 2.418493 7.829539
H 7.891948 1.981589 6.848578
H 6.605911 2.723765 7.827256
H 7.785538 1.637062 8.594035
C 8.363241 4.680780 7.022820
H 8.940224 5.592380 7.222182
H 7.301001 4.957934 6.972175
H 8.660844 4.286733 6.042095
C 8.190969 4.215558 9.490565
H 8.374379 3.490967 10.295391
H 7.123370 4.477652 9.501302
H 8.763036 5.127458 9.701486
C 13.560983 2.852718 7.875883
C 14.061033 3.017668 6.432479
H 13.700108 2.187081 5.806732
H 15.160496 3.007761 6.416269
H 13.720243 3.971895 6.007412
C 14.090759 3.992685 8.759137
H 13.902937 4.985360 8.334761
H 15.178699 3.871212 8.851057
H 13.659164 3.953865 9.768996
C 14.070293 1.520358 8.446943
H 13.741760 1.383859 9.487337
H 15.168759 1.516069 8.431040
H 13.720398 0.673883 7.835498
C 8.760378 -2.028761 4.051118
H 9.788584 -2.331509 3.804958
H 8.403112 -1.349489 3.263138
H 8.120014 -2.924949 4.045829
C 9.117885 -2.503079 7.068366
H 8.555522 -3.428288 6.865142
H 8.848794 -2.165719 8.080226
H 10.192903 -2.735392 7.049626
C 6.930103 -0.601008 6.056185
H 6.235015 -1.441195 5.896661
H 6.643708 0.207190 5.367935
H 6.788045 -0.240732 7.084886
C 8.202003 2.314023 3.556059
H 7.759511 2.799839 4.437475
H 7.626359 1.398937 3.353117
H 8.071869 2.991186 2.696699
C 10.999516 3.534575 3.983607
H 12.063747 3.339994 4.175618
H 10.601622 4.133591 4.814540
H 10.916189 4.134767 3.064163
C 10.666094 1.021842 2.248755
H 10.601003 1.685090 1.371603
H 10.076062 0.117171 2.041982
H 11.712281 0.711933 2.386897
C 10.819486 0.256314 9.114736
H 11.759623 -0.295007 8.939516
C 8.855180 0.556587 11.456760
H 8.730115 0.748737 12.533195
H 8.448450 -0.444047 11.244362
H 8.239889 1.289128 10.914128
C 11.644312 -0.663683 11.899905
H 12.711367 -0.627454 11.632193
H 11.273493 -1.671646 11.660498
H 11.562137 -0.519240 12.987968
C 11.348979 2.351905 11.431978

H 10.771945 3.151778 10.948511
H 12.404376 2.470818 11.149528
H 11.274655 2.492539 12.521039
N 9.946927 3.093922 8.138720
N 12.072061 2.783104 7.865787
Si 10.769985 1.479996 7.703642
Si 10.419014 0.452737 5.628401
Si 8.705830 -1.204057 5.755426
Si 10.042339 1.910950 3.793609
Si 10.674307 0.653523 10.962623
H 10.032008 -0.482132 8.884410
Te 12.576856 -0.748508 5.490393

(17) Ph_3P

34

P 1.210352 -0.022921 -0.121410
C 0.532807 0.768072 1.399647
C 1.207772 0.510684 2.605776
C -0.592314 1.606613 1.420496
C 0.756108 1.060348 3.806444
C -1.035168 2.168870 2.620877
C -0.366005 1.894665 3.816377
H 2.095217 -0.127528 2.601031
H -1.126505 1.821959 0.493411
H 1.288144 0.845549 4.735230
H -1.910585 2.821503 2.620590
H -0.713333 2.335024 4.752801
C 0.290326 0.860948 -1.452290
C 0.795587 2.110692 -1.853383
C -0.854936 0.359545 -2.089499
C 0.157720 2.850477 -2.849849
C -1.484030 1.094051 -3.099034
C -0.983805 2.341993 -3.478464
H 1.695748 2.507126 -1.376785
H -1.259491 -0.610059 -1.794778
H 0.558171 3.822547 -3.144008
H -2.373134 0.689028 -3.586460
H -1.477600 2.914944 -4.265414
C 0.375623 -1.666297 -0.104317
C 0.858891 -2.635222 -1.001061
C -0.690188 -2.002407 0.744388
C 0.275928 -3.901750 -1.063649
C -1.264513 -3.275494 0.690848
C -0.787231 -4.226111 -0.215082
H 1.699199 -2.391947 -1.656381
H -1.075265 -1.264698 1.450484
H 0.659346 -4.641215 -1.769328
H -2.092679 -3.522524 1.358222
H -1.237812 -5.219501 -0.256020

(18) **Tri-membered ring of S**

85

C 11.044882 3.807402 8.192862
C 11.338611 5.255961 8.366162
C 11.553023 6.047924 7.228095
H 11.496835 5.593424 6.238395
C 11.834842 7.407970 7.358605
H 11.992820 8.014147 6.465183
C 11.921745 7.987267 8.627151
H 12.151142 9.049215 8.729525
C 11.716558 7.201025 9.764311
H 11.789224 7.645284 10.758399
C 11.419428 5.843897 9.635563
H 11.270448 5.233441 10.526642
C 8.513798 3.769232 8.460673
C 7.542406 2.578089 8.501490
H 7.643263 1.964527 7.596607
H 6.507509 2.942478 8.562113
H 7.735696 1.938845 9.372092
C 8.186460 4.633569 7.229585
H 8.842250 5.512515 7.169646
H 7.146211 4.987200 7.280805
H 8.306333 4.042125 6.311306
C 8.332607 4.592842 9.747828
H 8.652442 4.015661 10.627344
H 7.269692 4.846573 9.872542
H 8.901957 5.529316 9.718432
C 13.413197 2.922430 7.643294
C 13.819163 3.187846 6.183497
H 13.375941 2.429707 5.523752
H 14.913956 3.151546 6.082049
H 13.479799 4.183605 5.864555
C 14.047484 3.984265 8.556662
H 13.860954 5.008562 8.214970
H 15.135214 3.826253 8.556967
H 13.691546 3.890215 9.591886
C 13.951395 1.549765 8.088627
H 13.696703 1.351715 9.138909
H 15.046573 1.540503 7.994307
H 13.545345 0.740810 7.469433
C 8.159003 -1.520273 3.795159
H 9.191307 -1.883197 3.684801
H 7.938356 -0.860064 2.943591
H 7.481646 -2.387386 3.739218
C 8.163533 -1.847265 6.856821
H 7.531359 -2.734199 6.693220
H 7.880365 -1.403572 7.822693
H 9.211384 -2.173856 6.923199
C 6.183012 0.102849 5.519159
H 5.443429 -0.705397 5.402469
H 6.009901 0.837962 4.720171
H 5.992320 0.598555 6.482051
C 7.798416 2.993566 3.211146

H 7.274377 3.494543 4.038596
H 7.211165 2.108366 2.925861
H 7.809943 3.681771 2.350989
C 10.562754 4.096386 3.997099
H 11.565195 3.859121 4.380223
H 10.054460 4.742664 4.726641
H 10.676556 4.664196 3.060169
C 10.371869 1.568990 2.261028
H 10.459044 2.211492 1.370532
H 9.783108 0.681120 1.987846
H 11.378622 1.230738 2.546770
C 10.562489 0.308726 8.977901
H 11.322231 -0.448990 8.729415
C 8.998569 0.763387 11.641463
H 9.095882 0.720495 12.737373
H 8.349201 -0.068223 11.328370
H 8.486684 1.704475 11.393918
C 11.606149 -0.840022 11.584580
H 12.618752 -0.935673 11.162604
H 11.066911 -1.776013 11.373217
H 11.701673 -0.741045 12.676637
C 11.664359 2.200988 11.318506
H 11.171133 3.098637 10.922508
H 12.700172 2.188210 10.953153
H 11.696845 2.286881 12.415633
N 9.874379 3.197275 8.358062
N 11.926118 2.882842 7.733489
Si 10.647191 1.551013 7.554700
Si 9.594432 1.076986 5.566116
Si 7.938491 -0.610637 5.443275
Si 9.569828 2.514801 3.690296
Si 10.707069 0.646245 10.839024
H 9.598036 -0.211891 8.843932
S 11.583685 0.223318 5.868881

(19) **Tri-membered ring of Se 85**

C 11.093710 3.829154 8.125384
C 11.381543 5.276029 8.311686
C 11.641693 6.070767 7.184924
H 11.626676 5.618397 6.192830
C 11.911186 7.431241 7.330666
H 12.103797 8.040778 6.446422
C 11.940918 8.007847 8.603508
H 12.159461 9.070817 8.718180
C 11.694818 7.217664 9.729369
H 11.727247 7.658943 10.726883
C 11.410105 5.859279 9.585251
H 11.238994 5.243334 10.468393
C 8.559692 3.803236 8.391297
C 7.564692 2.649037 8.194378
H 7.626677 2.247256 7.174722
H 6.540040 3.008736 8.361679
H 7.761151 1.826781 8.895541
C 8.292256 4.865386 7.311006
H 8.921889 5.754256 7.442979
H 7.241089 5.184450 7.358572
H 8.478302 4.449193 6.311606
C 8.341203 4.414478 9.786700
H 8.584286 3.690773 10.576385
H 7.286766 4.705575 9.901571
H 8.955426 5.310900 9.932893
C 13.472902 2.948190 7.639534
C 13.921385 3.204791 6.191335
H 13.503143 2.438811 5.523601
H 15.019016 3.173359 6.124885
H 13.586313 4.195889 5.854135
C 14.073695 4.017645 8.566778
H 13.899393 5.040202 8.214429
H 15.160634 3.859367 8.603609
H 13.684700 3.927454 9.590814
C 14.003106 1.584232 8.117079
H 13.730983 1.405659 9.166959
H 15.099606 1.575479 8.041682
H 13.607311 0.766070 7.502517
C 8.176875 -1.615422 3.916427
H 9.215591 -1.951368 3.783489
H 7.910183 -0.984940 3.055483
H 7.522581 -2.501552 3.906952
C 8.237768 -1.863892 6.986217
H 7.587875 -2.745054 6.866483
H 7.988279 -1.389552 7.947161
H 9.281824 -2.206858 7.027055
C 6.221437 0.030767 5.638985
H 5.491912 -0.787073 5.524688
H 6.031533 0.766489 4.844441
H 6.032281 0.518562 6.605961
C 7.715113 3.102019 3.434125
H 7.294415 3.591963 4.324364
H 7.058513 2.259597 3.172009
H 7.684341 3.824361 2.602819
C 10.611909 4.016510 3.984154
H 11.622549 3.700438 4.278704
H 10.210849 4.673575 4.768561
H 10.687936 4.603377 3.055302
C 10.091079 1.574335 2.191114
H 10.131218 2.244404 1.317734
H 9.422196 0.735473 1.949436
H 11.097256 1.164957 2.364419
C 10.757757 0.310482 8.911673
H 11.708065 -0.221302 8.745720

C 8.839191 0.626846 11.353300
H 8.794005 0.634974 12.453370
H 8.314431 -0.275801 11.003927
H 8.280473 1.501492 10.993169
C 11.511871 -0.828529 11.613351
H 12.573640 -0.866263 11.325291
H 11.053146 -1.786572 11.324825
H 11.460557 -0.743743 12.709649
C 11.476067 2.215568 11.342508
H 10.976193 3.095073 10.915435
H 12.534741 2.246902 11.046468
H 11.431521 2.295958 12.439374
N 9.917091 3.219704 8.272361
N 11.981487 2.904434 7.683532
Si 10.692441 1.578564 7.515279
Si 9.658506 1.011275 5.541196
Si 7.982680 -0.666609 5.544048
Si 9.494715 2.511958 3.721730
Si 10.637569 0.622150 10.775033
H 9.984385 -0.436667 8.665998
Se 11.771404 0.086313 5.645019

(20) **$Si(SiMe_3)_2$**

27

C 0.562594 -1.613218 -0.650464
H -0.098503 -2.408815 -0.276645
H 1.596657 -1.867998 -0.382303
H 0.481703 -1.601245 -1.749623
C -1.660365 0.507505 -0.664170
H -1.647959 0.528872 -1.765817
H -2.002663 1.491280 -0.309875
H -2.400313 -0.240443 -0.343044
C 1.251466 1.415409 -0.655023
H 1.182104 1.441575 -1.754589
H 2.296711 1.215542 -0.383271
H 0.987399 2.414923 -0.279387
C 2.596333 1.823430 2.981665
H 1.909022 2.318887 3.682695
H 2.499351 2.308654 2.000659
H 3.623186 1.988374 3.346752
C 2.631051 -0.799156 4.589126
H 2.455504 -1.885490 4.591499
H 1.980150 -0.353050 5.355345
H 3.679125 -0.625587 4.881570
C 3.532193 -0.830025 1.679134
H 4.553283 -0.663915 2.058985
H 3.469532 -0.400661 0.670293
H 3.378715 -1.916172 1.597553
Si -0.051700 -0.178257 2.393141
Si 0.060856 0.098575 0.018889
Si 2.283371 -0.054794 2.880169

(21) **4**

58

C -1.134737 0.937718 0.232876
C -1.787528 1.425516 -1.008141
C -1.234701 2.484913 -1.739557
H -0.321360 2.967666 -1.389736
C -1.856427 2.922090 -2.910819
H -1.422506 3.749190 -3.474728
C -3.026752 2.303755 -3.357699
H -3.508474 2.645247 -4.275276
C -3.580531 1.248016 -2.627293
H -4.494910 0.762579 -2.971829
C -2.966332 0.810579 -1.454309
H -3.399031 -0.010654 -0.880845
C 0.729242 -0.578899 -0.712096
C 1.445331 -1.745266 -0.013548
H 2.012814 -1.386118 0.858448
H 2.151612 -2.219089 -0.708687
H 0.725963 -2.506017 0.318688
C 1.775988 0.455377 -1.168089
H 1.298967 1.281074 -1.713649
H 2.506140 -0.019352 -1.840073
H 2.305191 0.867298 -0.297816
C -0.058467 -1.110486 -1.918054
H -0.841207 -1.813640 -1.603240
H 0.633136 -1.645013 -2.584747
H -0.524321 -0.303104 -2.496178
C -2.179480 2.473496 2.012829
C -1.365321 3.747170 1.716624
H -0.342863 3.639994 2.104972
H -1.840425 4.617058 2.193315
H -1.315436 3.938496 0.635711
C -3.590731 2.593851 1.420162
H -3.569872 2.824345 0.348122
H -4.122999 3.409765 1.929609
H -4.164786 1.668630 1.567407
C -2.276075 2.277446 3.533586
H -2.857756 1.378632 3.779151
H -2.771855 3.144874 3.989859
H -1.272587 2.184111 3.976029
C -0.665389 -1.253704 3.042272
H -0.730683 -0.951664 4.103582
C -2.224496 -3.772304 3.746231
H -3.122472 -4.385836 3.576477
H -2.201286 -3.492964 4.810410
H -1.342520 -4.398677 3.544227
C -3.791777 -1.241032 3.018140
H -3.882758 -0.376519 2.346067
H -3.797690 -0.870215 4.053823
H -4.683893 -1.871474 2.881629
C -2.302384 -2.795854 0.844471

H -1.432057 -3.412822 0.576450
H -2.331813 -1.938722 0.157184
H -3.206357 -3.399888 0.672271
N -0.138938 0.040854 0.311595
N -1.447324 1.293974 1.494746
Si -0.037720 0.273445 2.153577
Si -2.233945 -2.237186 2.645817
H 0.185908 -1.958792 3.009060
S 1.565594 1.240935 2.870878

(22) **5**

58

C -1.130757 0.939068 0.229124
C -1.773448 1.435646 -1.013430
C -1.209063 2.495421 -1.735587
H -0.295434 2.970808 -1.376687
C -1.819961 2.942330 -2.908853
H -1.376884 3.769549 -3.465345
C -2.990572 2.332938 -3.367259
H -3.463821 2.681677 -4.286520
C -3.555610 1.276616 -2.646300
H -4.470248 0.798344 -2.999979
C -2.952589 0.829675 -1.471034
H -3.394196 0.007953 -0.905157
C 0.725641 -0.589617 -0.713229
C 1.440759 -1.754467 -0.011492
H 2.011102 -1.392874 0.857697
H 2.144964 -2.231667 -0.706407
H 0.721027 -2.512878 0.325328
C 1.773707 0.438297 -1.179639
H 1.297800 1.263603 -1.726641
H 2.497769 -0.043188 -1.853343
H 2.309676 0.851688 -0.314122
C -0.070290 -1.124709 -1.912158
H -0.858517 -1.817873 -1.589004
H 0.614561 -1.671613 -2.575644
H -0.529997 -0.317916 -2.496045
C -2.186902 2.469092 2.009322
C -1.390236 3.752099 1.707304
H -0.365907 3.660820 2.095017
H -1.876927 4.616601 2.182095
H -1.344282 3.941127 0.625926
C -3.600954 2.569533 1.419336
H -3.585010 2.800854 0.347431
H -4.143754 3.377600 1.930089
H -4.161897 1.636313 1.566998
C -2.276927 2.276509 3.530752
H -2.847986 1.372346 3.781451
H -2.781122 3.140094 3.985050
H -1.271155 2.196321 3.970951
C -0.664630 -1.254044 3.047596
H -0.724638 -0.948574 4.108081
C -2.204992 -3.783202 3.746740
H -3.103665 -4.397822 3.585142
H -2.166987 -3.512296 4.812659
H -1.324387 -4.405462 3.526828
C -3.790108 -1.250124 3.058270
H -3.893954 -0.383791 2.390425
H -3.782913 -0.882831 4.095174
H -4.681904 -1.882981 2.931776
C -2.321681 -2.780769 0.853703
H -1.451620 -3.390709 0.569409
H -2.363558 -1.916777 0.175704
H -3.224651 -3.387489 0.686007
N -0.139167 0.037119 0.310317
N -1.443876 1.295299 1.491379
Si -0.040688 0.269111 2.150224
Si -2.235184 -2.239657 2.659151
H 0.187651 -1.957675 3.012724
Se 1.686083 1.299352 2.914582

(23) **$Si_2(SiMe_3)_4$**

54

C 0.447031 -4.209707 0.614718
H -0.530123 -4.538888 0.993412
H 1.222843 -4.755256 1.171721
H 0.522137 -4.496017 -0.446465
C -0.581683 -1.403979 -0.248106
H -0.483157 -1.709826 -1.301850
H -0.399508 -0.321307 -0.187207
H -1.618007 -1.586342 0.062284
C 2.390606 -1.878065 0.144675
H 2.454500 -2.154171 -0.920089
H 3.202110 -2.397183 0.673382
H 2.569823 -0.796045 0.222914
C 3.797560 -0.423936 3.495352
H 3.405048 0.573037 3.741828
H 3.913301 -0.482254 2.404058
H 4.796785 -0.520273 3.949283
C 2.582032 -1.655789 6.032456
H 1.822754 -2.327039 6.457232
H 2.360001 -0.631211 6.357254
H 3.561664 -1.939308 6.448852
C 3.389100 -3.475748 3.715150
H 4.396881 -3.566338 4.151865
H 3.477972 -3.626165 2.630023
H 2.768039 -4.288593 4.118434
Si 0.547194 -1.687584 3.082208
Si 0.676042 -2.340554 0.811898
Si 2.652086 -1.781993 4.150046
Si -1.394706 -1.390551 4.047567
Si -1.787466 -0.325575 6.119236
Si -3.419270 -1.831351 2.903242

C	-3.038489	1.058972	5.774756
H	-3.971694	0.679276	5.337069
H	-3.291173	1.573091	6.715973
H	-2.618642	1.802771	5.082342
C	-2.534803	-1.538958	7.365634
H	-1.828325	-2.349379	7.595285
H	-2.774913	-1.018036	8.306442
H	-3.459127	-1.993587	6.983269
C	-0.260676	0.471201	6.894120
H	-0.579728	1.138251	7.710675
H	0.414226	-0.282904	7.318228
H	0.301920	1.069583	6.164064
C	-3.305076	-3.376854	1.817033
H	-2.585665	-3.268185	0.995564
H	-3.004357	-4.248085	2.416599
H	-4.291473	-3.590043	1.374919
C	-3.968478	-0.347296	1.863426
H	-4.103317	0.543719	2.493799
H	-3.226181	-0.100623	1.091676
H	-4.927313	-0.561645	1.364513
C	-4.761808	-2.187453	4.195592
H	-5.709887	-2.412004	3.681276
H	-4.499109	-3.059078	4.812244
H	-4.938128	-1.336334	4.866803

(24) (**6**)$_2$ (gas phase)
170

Te	5.246799	14.752203	2.504096
Si	7.634442	12.460105	3.897622
Si	5.919037	12.383050	2.313885
Si	6.540817	11.741445	0.116876
Si	4.067667	11.088899	3.081195
Si	7.967829	12.483887	7.243288
N	9.172217	13.422238	3.536909
N	9.079281	11.277806	3.823121
C	11.030187	15.095547	3.841430
H	11.244817	14.669962	4.832148
H	11.190719	16.180505	3.896330
H	11.751954	14.692408	3.122178
C	9.570085	14.855112	3.427594
C	9.341807	15.322986	1.982570
H	9.988702	14.769560	1.287273
H	9.584379	16.391090	1.896112
H	8.288663	15.179001	1.696636
C	11.678666	12.361688	1.731301
H	10.903458	12.571817	0.994057
C	8.662990	15.650156	4.378469
H	7.602264	15.519500	4.112767
H	8.902197	16.718618	4.298616
H	8.819997	15.347650	5.423674
C	12.325191	11.913654	4.023213
H	12.060200	11.804100	5.075271
C	13.660469	11.833630	3.627208
H	14.433324	11.641537	4.373110
C	13.013282	12.267658	1.338495
H	13.276515	12.405843	0.288855
C	9.777915	9.402121	2.319848
H	9.132426	9.799836	1.525643
H	9.782272	8.305939	2.238720
H	10.802144	9.755951	2.148652
C	9.252488	9.811231	3.705267
C	9.829421	12.742101	7.072041
H	10.074484	13.750968	6.711060
H	10.261264	12.013031	6.373142
H	10.320992	12.607738	8.047413
C	11.326264	12.179245	3.077036
C	7.856981	9.209729	3.910887
H	7.444960	9.490429	4.891566
H	7.903629	8.113589	3.865130
H	7.161984	9.554333	3.133078
C	9.902985	12.292721	3.483461
C	5.350204	12.610252	-1.061701
H	5.354017	13.693016	-0.869738
H	4.319421	12.253821	-0.924872
H	5.642424	12.430659	-2.108296
C	14.006963	12.006357	2.285144
H	15.051853	11.942510	1.978006
C	7.009214	12.760899	5.633184
H	6.077638	12.174099	5.710301
H	6.660115	13.807481	5.597483
C	8.308777	12.281169	-0.298853
H	8.530713	12.085486	-1.359446
H	9.039952	11.727336	0.306305
H	8.442301	13.355408	-0.109879
C	4.324054	9.215641	3.265743
H	4.968377	8.971811	4.122304
H	4.766045	8.764536	2.365918
H	3.347917	8.733775	3.436708
C	7.299876	13.704699	8.514881
H	6.213005	13.589109	8.641355
H	7.489600	14.741758	8.198715
H	7.772949	13.560093	9.497953
C	3.419209	11.764124	4.724339
H	2.376825	11.442829	4.875939
H	3.449467	12.863646	4.720104
H	4.006635	11.399069	5.579932
C	6.403452	9.864929	-0.143402
H	5.364324	9.530114	-0.010046
H	7.030093	9.294761	0.557720
H	6.713543	9.595763	-1.165544
C	10.197603	9.287918	4.800035

H	11.225096	9.639311	4.643331
H	10.212076	8.188890	4.781779
H	9.863204	9.609929	5.795262
C	2.756196	11.371348	1.744835
H	1.787234	10.963328	2.072977
H	3.029038	10.877194	0.800607
H	2.633853	12.446524	1.549216
C	7.649573	10.721023	7.841636
H	8.153908	10.535369	8.802070
H	8.013144	9.969960	7.125578
H	6.573285	10.545515	7.990809
Te	9.415574	24.353327	3.785296
Si	7.209111	21.895867	2.198557
Si	8.917779	21.942589	3.800466
Si	8.327952	21.127737	5.946908
Si	10.857771	20.841478	2.967815
Si	6.935519	21.914101	-1.156011
N	5.632200	22.805032	2.527134
N	5.813111	20.663374	2.257454
C	3.720774	24.404590	2.189974
H	3.551422	23.978081	1.190851
H	3.518715	25.482989	2.135275
H	2.995616	23.966035	2.884908
C	5.177256	24.218311	2.644250
C	5.344463	24.679737	4.100252
H	4.699997	24.094198	4.771287
H	5.061140	25.738477	4.191304
H	6.394641	24.578597	4.415605
C	3.155371	21.622574	4.313224
H	3.918302	21.841708	5.060662
C	6.080808	25.058793	1.728656
H	7.137015	24.964740	2.026577
H	5.801346	26.117983	1.815430
H	5.964817	24.758133	0.677161
C	2.541761	21.193877	2.008928
H	2.819289	21.105149	0.958387
C	1.207443	21.058961	2.392888
H	0.448394	20.847483	1.638209
C	1.821964	21.474813	4.693736
H	1.547089	21.581141	5.744122
C	5.156960	18.729418	3.706287
H	5.776080	19.137629	4.516398
H	5.194772	17.631479	3.762610
H	4.117131	19.038798	3.870373
C	5.682407	19.186084	2.336507
C	5.066152	22.133220	-1.021243
H	4.794105	23.139612	-0.672915
H	4.638112	21.400496	-0.323812
H	4.594988	21.979421	-2.003859
C	3.523438	21.477543	2.967429
C	7.093997	18.625951	2.128687
H	7.505218	18.937932	1.157086
H	7.059966	17.527484	2.147634
H	7.774973	18.970072	2.919975
C	4.946046	21.645134	2.576973
C	9.490730	21.954658	7.183403
H	9.473342	23.045171	7.041733
H	10.528260	21.618895	7.044810
H	9.186410	21.722062	8.216093
C	0.845162	21.195435	3.734966
H	-0.198535	21.085262	4.033086
C	7.856543	22.211235	0.471533
H	8.796035	21.635032	0.410898
H	8.191269	23.262694	0.514989
C	6.544997	21.599546	6.381365
H	6.317777	21.342025	7.427500
H	5.832134	21.064215	5.738843
H	6.392581	22.679965	6.248608
C	10.684753	18.990577	2.568559
H	10.036071	18.820926	1.697576
H	10.258788	18.439727	3.419558
H	11.673072	18.558178	2.343081
C	7.601025	23.149431	-2.417229
H	8.691892	23.054242	-2.525486
H	7.387318	24.182884	-2.104872
H	7.147546	22.995497	-3.408219
C	11.534412	21.717917	1.434599
H	12.594235	21.455163	1.289953
H	11.455126	22.807406	1.563749
H	10.991737	21.436325	0.520473
C	8.515693	19.242745	6.108142
H	9.553250	18.937146	5.906193
H	7.861830	18.695910	5.414024
H	8.263287	18.917485	7.130087
C	4.764201	18.662467	1.220109
H	3.721921	18.963355	1.384523
H	4.799112	17.562949	1.201296
H	5.088674	19.033096	0.238134
C	12.125170	21.014683	4.365503
H	13.118603	20.684520	4.022877
H	11.847872	20.407826	5.240096
H	12.197920	22.064806	4.683659
C	7.307196	20.162125	-1.753651
H	6.833316	19.971844	-2.728625
H	6.940980	19.398463	-1.052979
H	8.390988	20.012395	-1.874508

(III) B3-LYP/6-31g(d) optimized geometries of compounds 2 and 6.

(1) **2**
84

C	-1.758961	-0.343246	H	-1.054834	-1.793980	H	0.436006	-3.804445
0.009947			3.915975			1.307623		
C	-3.085816	-1.014374	H	-2.036907	-2.123397	H	0.873809	-4.810033
0.147646			2.483103			0.083925		
C	-3.177840	-2.409876	C	-2.154172	0.589986	C	2.873076	-2.946232
0.041822			3.042748			1.796074		
H	-2.283505	-2.999375	H	-3.117857	0.191358	H	2.959470	-4.000635
0.134016			2.716226			2.093667		
C	-4.415512	-3.042772	H	-2.120490	0.527639	H	3.842574	-2.469253
0.166521			4.136258			1.983571		
H	-4.474792	-4.124148	H	-2.100686	1.646664	H	2.142578	-2.471828
0.084253			2.761735			2.461781		
C	-5.569258	-2.290709	C	0.341713	0.352377	C	0.607180	2.395880
0.394913			3.017742			0.357066		
H	-6.531868	-2.784914	H	0.463722	1.414561	H	1.506099	2.609149
0.489821			2.781265			0.240592		
C	-5.482167	-0.901053	H	0.343922	0.248238	C	-0.186640	5.269855
0.499758			4.107422			1.031615		
H	-6.376042	-0.309037	H	1.204858	-0.189992	H	-0.817624	6.136578
0.673772			2.620410			0.798308		
C	-4.247374	-0.263663	C	4.019701	1.063485	H	0.858493	5.573960
0.377302			1.798529			0.896370		
H	-4.188826	0.817904	H	3.180127	1.737604	H	-0.326388	5.034629
0.443439			2.007649			2.094037		
C	-1.586944	-0.186567	H	3.897081	0.179528	C	-0.400549	4.313813
2.584899			2.435470			1.878203		
C	-0.766367	0.812541	H	4.940502	1.576085	H	-0.653682	3.515042
3.421726			2.110058			2.584493		
H	0.307756	0.649033	C	4.436182	2.187795	H	0.635559	4.614396
3.287661			1.019444			2.077043		
H	-0.999124	0.679872	H	5.331262	2.694499	H	-1.042442	5.172457
4.483284			0.633655			2.111606		
H	-1.005839	1.845744	H	4.602141	1.975635	C	-2.441137	3.348184
3.147679			2.082255			0.222147		
C	-1.238607	-1.622473	H	3.600625	2.893850	H	-2.617864	3.000723
3.024071			0.952732			1.245834		
H	-1.824771	-2.358803	C	5.684717	-0.482003	H	-2.775408	2.563096
2.465248			0.241574			0.464241		
H	-1.460430	-1.752628	H	6.567798	0.090658	H	-3.074783	4.227913
4.089548			0.072082			0.054782		
H	-0.174521	-1.823262	H	5.645259	-1.391054	N	-1.183717	0.018958
2.865616			0.370030			1.167203		
C	-3.082967	0.091877	H	5.838433	-0.788602	N	-0.897542	-0.019607
2.820111			1.282883			0.971994		
H	-3.368986	1.075998	C	3.695826	-3.793316	Si	0.407809	0.507047
2.434412			1.013661			0.295117		
H	-3.274884	0.082820	H	3.438402	-3.855083	Si	2.291297	-0.631696
3.898649			2.077625			1.011578		
H	-3.727419	-0.661280	H	4.687946	-3.332798	Si	4.104073	0.574721
2.363058			0.942584			0.049742		
C	-0.974399	-0.201297	H	3.774673	-4.817836	Si	2.380325	-2.800296
2.444912			0.625179			0.047580		
C	-1.094021	-1.689725	C	0.748378	-3.773835	Si	-0.621986	3.787872
2.825782			0.257458			0.069769		
H	-0.267904	-2.266288	H	-0.067994	-3.331617	H	0.930108	2.574214
2.399411			0.324459			1.394192		

(2) **6**

85

Te	-2.878543	-0.267706	-2.213573
Si	0.133179	0.618073	0.007652
Si	-2.011498	-0.429535	0.135440
Si	-1.981870	-2.687747	0.907121
Si	-3.482568	0.872854	1.510677
Si	1.320685	3.828388	-0.081863
N	1.456224	-0.134535	-1.064805
N	1.567054	0.100327	1.083984
C	3.188565	-0.279676	-2.896095
H	3.639547	0.647444	-2.526939
H	3.266383	-0.278235	-3.988305
H	3.771997	-1.124370	-2.526300
C	1.696121	-0.369095	-2.524561
C	1.130938	-1.745766	-2.920376
H	1.651500	-2.552112	-2.393375
H	1.266243	-1.903392	-3.996456
H	0.059906	-1.802301	-2.701874
C	3.475959	-2.569848	-0.091569
H	2.529974	-3.093770	-0.181338
C	0.943674	0.735157	-3.287470
H	-0.131394	0.702732	-3.080539
H	1.075962	0.582171	-4.363510
H	1.337175	1.726557	-3.036889
C	4.720609	-0.503525	0.144249
H	4.744740	0.579161	0.210771
C	5.914302	-1.225667	0.138923
H	6.860228	-0.698266	0.219243
C	4.672742	-3.287355	-0.087503
H	4.649011	-4.369420	-0.176251
C	2.008018	-1.483679	2.981844
H	1.133244	-2.073717	2.692265
H	2.100840	-1.528010	4.072620
H	2.898605	-1.949109	2.553095
C	1.853478	-0.015437	2.541476
C	3.065280	3.254773	-0.547316
H	3.117619	2.888657	-1.578872
H	3.413721	2.455410	0.115661
H	3.771325	4.089765	-0.458162
C	3.493596	-1.172304	0.029840
C	0.643568	0.598779	3.262343
H	0.492052	1.642268	2.964713
H	0.804647	0.580502	4.344579
H	-0.272096	0.039543	3.050472
C	2.209821	-0.411755	0.012570
C	-3.539923	-3.541278	0.240874
H	-3.580579	-3.471080	-0.850933
H	-4.453969	-3.082102	0.633260
H	-3.543595	-4.602324	0.524058
C	5.893008	-2.617503	0.025882
H	6.823556	-3.177558	0.023504
C	-0.012713	2.474985	-0.266645
H	-0.854007	2.794016	0.365814
H	-0.416479	2.543740	-1.287649
C	-0.473188	-3.659073	0.270077
H	-0.559522	-4.718043	0.546280
H	0.463286	-3.280728	0.695031
H	-0.402482	-3.601396	-0.821552
C	-2.954145	1.151178	3.323070
H	-2.078829	1.805457	3.402743
H	-2.723432	0.212655	3.839827
H	-3.775249	1.635095	3.868824
C	0.824797	5.257263	-1.222644
H	-0.179496	5.627830	-0.984124
H	0.820395	4.948648	-2.275192
H	1.521783	6.099132	-1.125932
C	-3.817916	2.580399	0.746575
H	-4.702745	3.031086	1.215186
H	-4.004474	2.493963	-0.328776
H	-2.980776	3.273882	0.890474
C	-2.022673	-2.826692	2.810991
H	-2.922009	-2.352271	3.221912
H	-1.154473	-2.366510	3.296527
H	-2.044940	-3.883390	3.109508
C	3.116959	0.782740	2.918764
H	4.018261	0.339977	2.488929
H	3.234531	0.786789	4.007986
H	3.041631	1.821081	2.581076
C	-5.118450	-0.098911	1.544555
H	-5.906493	0.505478	2.012821
H	-5.027315	-1.028444	2.119120
H	-5.443368	-0.356517	0.530961
C	1.332906	4.463683	1.704594
H	2.041063	5.294851	1.811480
H	1.623325	3.692413	2.427159
H	0.343488	4.836113	1.9975