Base-Stabilized Acyclic Amino(ylidyl)silylenes: Electron-Rich Donors for the Stabilization of Silicon-Element Multiple Bonds

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1 General Experimental Details

All experiments were carried out under a dry, oxygen-free argon atmosphere using standard Schlenk techniques. Involved solvents were dried using an MBraun SPS-800 (THF, DCM, toluene, acetonitrile, diethylether, hexane and pentane). Deuterated solvents were degassed and stored over molecular sieves in an argon-filled glovebox. ^{Ts}**Y'-Na**,[27a] ^{Ts}**Y-Li**,[22] ^{CN}**Y-K**,[27b] and Roesky's chlorosilylene **1**[26b] were prepared according to literature procedures. All other reagents were purchased from Sigma-Aldrich, ABCR, Rockwood Lithium or Acros Organics and used without further purification.

NMR spectra were recorded on Avance-400 spectrometers at 25 °C if not stated otherwise. All values of the chemical shift are in ppm regarding the δ-scale. All spin-spin coupling constants (*J*) are printed in Hertz (Hz). To display multiplicities and signal forms correctly the following abbreviations were used: s = singlet, d = doublet, t = triplet m = multiplet, dd = doublet of doublet, br = broad signal. Signal assignment was supported by APT, HSQC (^{1}H / ^{13}C) and HMBC (^{1}H / ^{13}C) correlation experiments.

IR-Spectra were recorded in an argon filled glovebox on a Shimadzu IRSpirit with QATR-S module and in transmission mode with a Specac "Omni-cell" with KBr plates and a 0.1 mm spacer. Measurement and processing details for individual spectra can be extracted from the corresponding tables in the supporting information.

Elemental analyses were performed on an Elementar vario MICRO-cube elemental analyzer.

HRMS-ESI: An LTQ Orbitrap Velos (Thermo Fisher Scientific, Bremen, Germany) was used for direct infusion via a syringe pump. The heated desolvation capillary was set to 200°C and a spray voltage of 1.8 kV was supplied. In the tune file the LTQ Orbitrap was set to the following parameters (R = 30,000; IT = 500 ms; AGC Target = 1,000,000).
HRMS-LIFDI: A JEOL AccuTof GCv (JMS-T100GCV) (JEOL, Tokyo, Japan) was equipped with a LIFDI source from Linden (CMS, Weyhe, Germany). The emitter heating current was set to 20 mA min^{-1} at a constant rate.

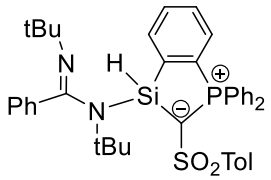
X-Ray data collection of the compounds was conducted with an Oxford Synergy. The structures were solved using dual space FT and direct methods, refined with the Shelx software package and expanded using Fourier techniques.[36-39] The crystals of all compounds were mounted in an inert oil (perfluoropolyalkylether). Crystal structure determination was affected at 100 K. Crystallographic data (including structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 2350308-2350312, 2366468 and 2366469. For explicit assignment, see chapter 5.1. Copies of the data can be obtained free of charge on application to Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; [fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk].

Safety comments
Caution! Metal bases such as organolithium bases, metal alkoxides or amides, especially as neat compounds, are severely air-/moisture-sensitive and pyrophoric organometallic compounds. These compounds need to be handled under an inert gas atmosphere to exclude reactions with oxygen and water. Guidelines for their handling can be found in literature: T. L. Rathman, J. A. Schwindeman, *Org. Process Res. Dev.* **2014**, *18*, 1192.

Caution! Carbon monoxide (CO) is a highly toxic gas. Reactions should be performed in well-ventilated fumehoods, ideally with a CO sensor.

2 Experimental Procedures

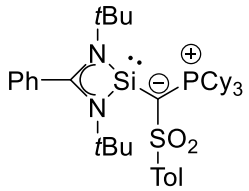
2.1 Synthesis of 2



307 mg (0.68 mmol, 1 eq.) **^{Ts}Y'-Li** and 200 mg (0.68 mmol, 1 eq.) PhC(N*t*Bu$_2$)$_2$SiCl (**1**) were dissolved in 10 mL diethyl ether at 0 °C. The reaction was allowed to warm to room temperature overnight and subsequently filtered. The reaction solution was concentrated and stored at -30 °C upon which yellow crystals formed. The crystals were filtered off and washed with cold pentane and dried *in vacuo* to obtain the product as a yellow solid (322 mg, 0.47 mmol, 69%). Single crystals suitable for X-ray diffraction analysis were formed while keeping the reaction solution at -30 °C in diethyl ether.

^{1}H-NMR (400.3 MHz, CD_2Cl_2): δ = 8.55 (dd, $^3J_{HH}$ = 7.5 Hz,$^4J_{HH}$ = 2.2 Hz, 1H, C*H*$_{SiPh,o}$), 7.87 – 7.77 (m, 3H, C*H*$_{SiPh,m+p}$), 7.63 – 7.54 (m, 6H, C*H*$_{PPh,o,\ CPh,o}$), 7.53 – 7.49 (m, 1H, C*H*$_{CPh,p}$), 7.49 – 7.42 (m, 6H, C*H*$_{PPh2,m+p}$), 7.41 – 7.36 (m, 2H, C*H*$_{CPh,m}$), 7.22 (d, $^3J_{HH}$ = 8.0 Hz, 2H, C*H*$_{Tol,o}$), 6.91 (d, $^3J_{HH}$ = 8.0 Hz, 2H, C*H*$_{Tol,m}$), 5.65 (d, $^3J_{HP}$ = 8.2 Hz, Si*H*), 2.25 (s, 1H, C*H*$_3$), 1.07 (s, 18H, C(C*H*$_3$)$_3$) ppm.
^{13}C{^{1}H}-NMR (100.7 MHz, CD_2Cl_2): δ = 163.1 (s, N*C*N), 149.9 (d, $^2J_{PC}$ = 19.8 Hz, Si*C*$_{Ph}$), 146.4 (s, *C*$_{Tol,ipso}$), 141.1 (s, *C*$_{Ph,ipso}$), 140.4 (s, *C*$_{Tol,p}$), 136.3 (d, $^3J_{PC}$ = 13.9 Hz, Si*C*$_{Ph,o}$), 134.4 (d, $^1J_{PC}$ = 98.1 Hz, SiC$_{Ph,o}$), 134.0 (d, $^2J_{PC}$ = 10.9 Hz, P*C*$_{Ph,o}$), 132.3 (s, *C*$_{Ph,o}$), 131.8 (d, $^4J_{PC}$ = 2.9 Hz, P*C*$_{Ph,p}$), 130.4 (s, Si*C*$_{Ph,m}$), 130.4 (d, $^2J_{PC}$ = 25.2 Hz, Si*C*$_{Ph,m}$), 130.3 (s, Si*C*$_{Ph,p}$), 129.0 (s, *C*$_{Ph,p}$) 128.9 (d, $^1J_{PC}$ = 86.0 Hz, P*C*$_{Ph,ipso}$), 128.8 (d, $^3J_{PC}$ = 12.6 Hz, P*C*$_{Ph,m}$), 128.7 (s, *C*$_{Tol,m}$), 127.6 (s, *C*$_{Ph,m}$), 126.1 (s, *C*$_{Tol,o}$), 55.4 (s, *C*(CH$_3$)$_3$), 44.4 (d, $^1J_{PC}$ = 84.1 Hz, P*C*Si), 32.4 (s, C(*C*H$_3$)$_3$), 21.3 (s, *C*H$_3$) ppm.
^{29}Si{^{1}H}-NMR (79.5 MHz, CD_2Cl_2): δ = -29.1 (d, $^2J_{PSi}$ = 34.7 Hz) ppm.
^{31}P{^{1}H}-NMR (162.0 MHz, C_6D_6): δ = 16.9 (s) ppm.
Elem. Anal. Calcd. for $C_{41}H_{45}N_2O_2PSSi$: C, 71.48; H, 6.58; N, 4.07; S, 4.65. Found: C, 71.29; H, 6.56; N, 3.99; S, 4.28.
HRMS-ESI (m/z): [M-H]$^+$ calcd for $C_{41}H_{46}N_2O_2PSSi$, 689.2776; found, 689.2787.

2.2 Synthesis of AYSi-2

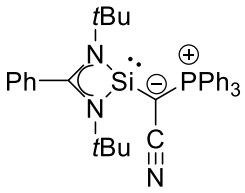


2.27 g (5.0 mmol, 1 eq.) Li[Cy$_3$PCSO$_2$Tol] and 1.47 g (5.0 mmol, 1 eq.) PhC(N*t*Bu$_2$)$_2$SiCl were dissolved in 150 mL toluene and stirred for 2 h at room temperature. The reaction mixture was filtered, and the volatiles were removed *in vacuo*. The residue was washed with 50 mL pentane and subsequently dried to yield the product as a yellow solid (3.07 g, 4.3 mmol, 87%). Single crystals suitable for X-ray diffraction analysis was obtained by pentane vapor diffusion into a saturated benzene solution of **AYSi-2**.

^{1}H-NMR (400.3 MHz, C_6D_6): δ = 8.35 (d, $^3J_{HH}$ = 7.8 Hz, 2H, C*H*$_{Tol,o}$), 7,68 (d, $^3J_{HH}$ = 7.6 Hz, 1H, C*H*$_{Ph,o}$), 7.12 (d, $^3J_{HH}$ = 7.8 Hz, 2H C*H*$_{Tol,m}$), 7.09 – 6.97 (m, 3H, C*H*$_{Ph,o+m}$), 6.95 – 6.87 (m, 1H, C*H*$_{Ph,p}$), 3.42 – 3.24 (m, 3H, C*H*$_{Cy,ipso}$), 2.30 – 2.15 (m, 6H, C*H*$_{Cy,m}$), 2.07 (s, 3H,

C$H_{3,Tol}$), 1.89 – 1.71 (m, 12H, C$H_{Cy,o}$), 1.69 – 1.57 (m, 4, C$H_{Cy,p}$), 1.42 – 1.15 (m, 26H, C$H_{Cy,m+p}$, C$H_{3,tBu}$) ppm.
^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6): δ = 157.1 (s, N*C*N), 150.5 (s, $C_{Tol,ipso}$), 139.3 (s, $C_{Tol,p}$), 136.0 (s, $C_{Ph,ipso}$), 131.3 (s, $C_{Ph,o}$), 129.3 (s, $C_{Tol,m}$), 129.0 (s, $C_{Tol,p}$), 128.5 (s, $C_{Tol,o}$), 127.2 (s, $C_{Ph,m}$), 53.8 (s, *C*(CH$_3$)$_3$), 48.1 (d, $^{1}J_{PC}$ = 58.6 Hz, P*C*Si), 35.2 (d, $^{1}J_{PC}$ = 48.7 Hz, P$C_{Cy,ipso}$), 32.0 (s, C(*C*H$_3$)$_3$), 28.8 (d, $^{3}J_{PC}$ = 6.2 Hz, P$C_{Cy,m}$), 27.7 (d, $^{2}J_{PC}$ = 6.2 Hz, P$C_{Cy,o}$), 26.7 (s, P$C_{Cy,p}$), 21.2 (s, *C*H$_{3,Tol}$) ppm.
^{29}Si{^{1}H}-NMR (79.5 MHz, C_6D_6): δ = 7.7 (d, $^{2}J_{PSi}$ = 44.7 Hz) ppm.
^{31}P{^{1}H}-NMR (162.0 MHz, C_6D_6): δ = 33.2 (s) ppm.
Elem. Anal. Calcd. for $C_{41}H_{63}N_2O_2PSSi$: C, 69.64; H, 8.98; N, 3.96; S, 4.53. Found: C, 64.49; H, 8.74; N, 3.63; S, 3.06. Repeated measurements always resulted in lower values for carbon and sulfur due to incomplete combustion.

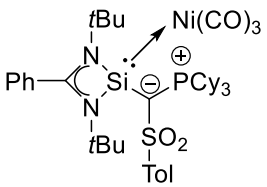
2.3 Synthesis of AYSi-3



0.83 g (2.81 mmol, 1 eq.) K[Ph$_3$PCCN] and 0.96 g (2.81 mmol, 1 eq.) PhC(N*t*Bu$_2$)$_2$SiCl were dissolved in 10 mL diethyl ether and stirred overnight at room temperature. The reaction mixture was filtered and the volatiles removed *in vacuo*. The residue was washed with twice with 5 mL pentane and dried. The product was obtained as an orange solid (1.23 g, 2.2 mmol, 78%). Single crystals suitable for X-ray diffraction analysis were obtained by storage of a saturated diethyl ether solution of **AYSi-3** at -30 °C.

^{1}H-NMR (400.3 MHz, C_6D_6): δ = 8.23 – 8.15 (m, 1H, C$H_{CPh,p}$), 7.93 – 7.82 (m, 6H, C$H_{PPh3,m}$), 7.10 – 7.01 (m, 9H, C$H_{PPh,o+pz}$), 7.00 – 6.89 (m, 4H, C$H_{CPh,o+m}$), 1.35 (s, 18H, C(CH_3)$_3$) ppm.
^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6): δ = 162.80 (s, N*C*N), 135.25 (s, $C_{CPh,ipso}$), 133.97 (d, $^{2}J_{PC}$ = 9.3 Hz, $C_{PPh3,o}$), 133.16 (s, $C_{CPh,ipso}$), 131.83 (d, $^{4}J_{PC}$ = 2.9 Hz, $C_{PPh3,p}$), 130.24 (s, $C_{CPh,o}$), 129.27 (d, $^{1}J_{PC}$ = 18.7 Hz, $C_{PPh3,ipso}$), 128.65 (d, $^{3}J_{PC}$ = 12.4 Hz, $C_{PPh3,m}$), 127.22 (s, $C_{Ph,m}$), 125.00 (d, $^{2}J_{PC}$ = 6.3 Hz, C*C*N), 53.01 (s, *C*(CH$_3$)$_3$), 31.71 (s, C(*C*H$_3$)$_3$), 15.87 (d, $^{1}J_{PC}$ = 106.8 Hz, *C*CN) ppm.
^{29}Si{^{1}H}-NMR (79.5 MHz, C_6D_6): δ = 23.68 (d, $^{2}J_{PSi}$ = 62.3 Hz) ppm.
^{31}P{^{1}H}-NMR (162.0 MHz, C_6D_6): δ = 24.9 (s) ppm.
HRMS-ESI (m/z): [M-H]$^+$ calcd for $C_{35}H_{39}N_3PSi$, 560.2632; found, 560.2650.

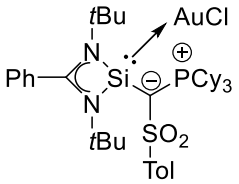
2.4 Synthesis of AYSi-2 nickel complex 3



70.6 mg (0.10 mmol, 1 eq.) **AYSI-2** was dissolved in 5 mL toluene and cooled to -30 °C and added to 27.5 mg (0.10 mmol, 1 eq.) Ni(COD)$_2$ at -30 °C in the dark. The solution was stirred for 5 minutes, and the reaction mixture was allowed to warm to room temperature. The volatiles were removed *in vacuo*. 5 mL pentane were added to the residue and the solution was filtered. The filtrate was dried *in vacuo* to yield the product as a colorless solid (60.0 mg, 0.07 mmol, 71%).
^{1}H-NMR (400.3 MHz, C_6D_6): δ = 8.36 (d, $^{3}J_{HH}$ = 8.2 Hz, 2H, C$H_{Tol,o}$), 7.88 (d, $^{3}J_{HH}$ = 8.4 Hz, C$H_{Ph,o}$), 7.57 (d, $^{3}J_{HH}$ = 7.6 Hz, C$H_{Ph,o}$), 6.97 – 6.87 (m, 5H, C$H_{Ph,m+p}$ + C$H_{Tol,m}$), 3.25 (q, $^{3}J_{HH}$ = 12.9 Hz, 3H,

C$H_{Cy,ipso}$), 2.31 – 2.18 (m, 6H, C$H_{Cy,p}$), 2.02 (s, 3H, C$H_{3,Tol}$), 1.70 – 1.41 (m, 30H, C$H_{Cy,o}$ + C(CH_3)$_3$), 1.38 – 1.20 (m, 8H, C$H_{Cy,m}$), 1.18 – 0.95 (m, 4H, C$H_{Cy,m}$) ppm.
^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6): δ = 202.7 (s, *C*O), 168.0 (s, N*C*N), 150.6 (s, $C_{Tol,ipso}$), 140.0 (s, $C_{Tol,p}$), 133.8 (s, $C_{Ph,ipso}$), 131.7k (s, $C_{Ph,o}$), 129.7 (s, $C_{Ph,p}$), 128.7 (s, $C_{Tol,m}$), 127.6 (s, $C_{Ph,m}$), 126.6 (s, $C_{Tol,o}$), 55.0 (s, *C*(CH$_3$)$_3$), 45.8 (d, $^1J_{PC}$ = 55.6 Hz, P*C*Si), 34.7 (d, $^1J_{PC}$ = 46.6 Hz, P$C_{Cy,ipso}$), 32.0 (s, C(*C*H$_3$)$_3$), 29.1 (d, $^3J_{PC}$ = 3.3 Hz, P$C_{Cy,m}$), 27.3 (d, $^2J_{PC}$ = 11.8 Hz, P$C_{Cy,o}$), 26.4 (s, P$C_{Cy,p}$), 21.1 (s, *C*H$_{3,Tol}$) ppm.
^{29}Si{^{1}H}-NMR (79.5 MHz, C_6D_6): δ = 63.0 (d, $^2J_{Psi}$ = 33.7 Hz) ppm.
^{31}P{^{1}H}-NMR (162.0 MHz, C_6D_6): δ = 31.9 (s) ppm.
Elem. Anal. Calcd. for $C_{44}H_{63}N_2NiO_5PSSi$: C, 62.19; H, 7.47; N, 3.30; S, 3.77. Found: C, 62.13; H, 7.30; N, 3.32; S, 2.48.

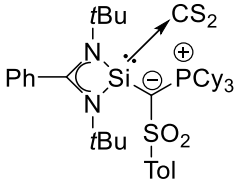
2.5 Synthesis of AYSi-2 gold complex 4



70.6 mg (0.10 mmol, 1 eq.) **AYSi-2** and 32.1 mg (0.10 mmol, 1 eq.) (THT)AuCl were dissolved in 5 mL toluene and stirred for one hour at room temperature. The reaction mixture was filtered over Celite, and the volatiles removed *in vacuo*. The product was obtained as a colourless solid (88.2 mg, 0.094 mmol, 94%).

^{1}H-NMR (400.3 MHz, C_6D_6): δ = 8.25 (d, $^3J_{HH}$ = 8.2 Hz, 2H, C$H_{Tol,o}$), 7.49 (d, $^3J_{HH}$ = 8.0 Hz, 1H, C$H_{Ph,p}$), 6.98 – 6.90 (m, 4H, C$H_{Ph,o+m}$), 6.97 – 6.90 (m, 2H C$H_{Tol,m}$), 3.60 – 3.40 (m, 2H, C$H_{Cy,ipso}$), 2.58 – 2.51 (m, 1H, C$H_{Cy,ipso}$), 2.03 (s, 3H, C$H_{3,Tol}$), 1.98 – 1.83 (m, 6H, C$H_{Cy,p}$), 1.64 – 1.35 (m, 34H, C$H_{Cy,o+m}$ + C(CH_3)$_3$), 1.29 – 0.96 (m, 8H, C$H_{Cy,m}$) ppm.
^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6): δ = 173.7 (s, N*C*N), 149.5 (s, $C_{Tol,ipso}$), 140.6 (s, $C_{Tol,p}$), 133.8 (s, $C_{Ph,ipso}$), 131.7 (s, $C_{Ph,p}$), 129.7 (s, $C_{Ph,o}$), 129.5 (s, $C_{Ph,o}$), 128.9 (s, $C_{Ph,m}$), 128.7 (s, $C_{Tol,o}$), 127.6 (s, $C_{Ph,m}$), 126.6 (s, $C_{Tol,m}$), 54.5 (s, *C*(CH$_3$)$_3$), 46.4 (d, $^1J_{PC}$ = 44.7 Hz, P*C*Si), 37.4 (d, $^1J_{PC}$ = 46.7 Hz, P$C_{Cy,ipso}$), 32.2 (s, C(*C*H$_3$)$_3$), 31.5 (d, $^1J_{PC}$ = 51.9 Hz, P$C_{Cy,ipso}$), 28.7 (br d, $^3J_{PC}$ = 3.2 Hz, P$C_{Cy,m}$), 27.4 (br d, $^2J_{PC}$ = 12.1 Hz, P$C_{Cy,o}$), 26.5 (s, P$C_{Cy,p}$), 21.1 (s, *C*H$_{3,Tol}$) ppm.
^{29}Si{^{1}H}-NMR (79.5 MHz, C_6D_6): δ = 28.1 (d, $^2J_{Psi}$ = 26.9 Hz) ppm.
^{31}P{^{1}H}-NMR (162.0 MHz, C_6D_6): δ = 31.0 (s) ppm.
Elem. Anal. Calcd. for $C_{41}H_{63}AuClN_2O_2PSSi$: C, 54.22; H, 6.76; N, 2.98; S, 3.41. Found: C, 54.18; H, 6.47; N, 2.56; S, 2.95.

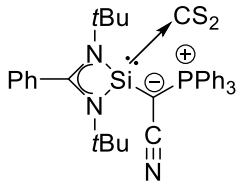
2.6 Synthesis of AYSi-2-CS_2 adduct 5_{Ts}



70.6 mg (0.10 mmol, 1 eq.) **AYSi-2** were dissolved in 3 ml of toluene and 6 µL CS_2 (0.10 mmol, 1. eq.) were added. The reaction mixture turned red and was stirred for 5 minutes at room temperature. The volatiles were removed *in vacuo* and the residue washed with 5 ml pentane. The remaining solid was dried *in vacuo* to yield the product as a purple powder (68.4 mg, 0.09 mmol, 87%). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a saturated dichloromethane solution of **5_{Ts}**.

^{1}H-NMR (400.3 MHz, C_6D_6): δ = 8.30 (d, $^{3}J_{HH}$ = 8.2 Hz, 2H, C$H_{Tol,o}$), 7.41 (d, $^{3}J_{HH}$ = 8.2, 1H, C$H_{Ph,p}$), 7.06 (d, 2H, $^{3}J_{HH}$ = 7.2 Hz, 1H, C$H_{Ph,o}$), 6.94 (d, $^{3}J_{HH}$ = 8.2 Hz, 2H C$H_{Tol,m}$), 6.88 (d, $^{3}J_{HH}$ = 7.2 Hz, 1H, C$H_{Ph,o}$), 6.85 – 6.78 (m, 2H, C$H_{Ph,m}$), 3.81 – 3.66 (m, 3H, C$H_{Cy,ipso}$), 2.39 – 2.28 (m, 6H, C$H_{Cy,m}$), 2.00 (s, 3H, C$H_{3,Tol}$), 1.63 – 1.53 (m, 24H, C$H_{Cy,m}$, C$H_{3,tBu}$), 1.45 – 1.29 (m, 12H, C$H_{Cy,o}$), 1.08 – 0.93 (m, 6H, C$H_{Cy,p}$) ppm.
^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6): δ = 273.3 (s, CS_2), 180.0 (s, NCN), 148.6 (s, $C_{Tol,ipso}$), 141.4 (s, $C_{Tol,p}$), 131.0 (s, $C_{Ph,ipso}$), 130.5 (s, $C_{Ph,o}$), 129.5 (s, $C_{Tol,p}$), 129.1 (s, $C_{Tol,o}$), 128.5 (s, $C_{Ph,m}$), 127.4 (s, $C_{Tol,m}$), 55.4 (s, $C(CH_3)_3$), 40.7 (d, $^{1}J_{PC}$ = 60.7 Hz, PCSi), 38.0 (d, $^{1}J_{PC}$ = 43.3 Hz, P$C_{Cy,ipso}$), 31.6 (s, C(CH_3)$_3$), 29.4 (d, $^{3}J_{PC}$ = 3.3 Hz, P$C_{Cy,m}$), 27.2 (d, $^{2}J_{PC}$ = 12.4 Hz, P$C_{Cy,o}$), 26.4 (s, P$C_{Cy,p}$), 21.1 (s, $CH_{3,Tol}$) ppm.
^{29}Si{^{1}H}-NMR (79.5 MHz, C_6D_6): δ = -39.4 (d, $^{2}J_{Psi}$ = 21.5 Hz) ppm.
^{31}P{^{1}H}-NMR (162.0 MHz, C_6D_6): δ = 32.8 (s) ppm.

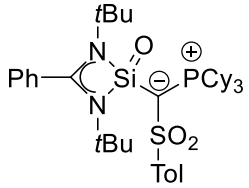
2.7 Synthesis of AYSi-3-CS_2 adduct 5_{CN}



56.1 mg (0.10 mmol, 1 eq.) **AYSi-3** were dissolved in 1 ml of C_6D_6 and 7.2 µL CS_2 (0.12 mmol, 1.2 eq.) were added. The reaction mixture turned red and was stirred for 5 minutes at room temperature. The reaction mixture was characterized by multinuclear NMR spectroscopy. Single crystals suitable for X-ray diffraction analysis were obtained by adding CS_2 to a concentrated solution of **AYSi-3** in toluene at -30 °C. The product could not be isolated.

^{1}H-NMR (400.3 MHz, C_6D_6): δ = 7.90 – 7.81 (m, 6H, C$H_{PPh,m}$), 7.47 (d, $^{3}J_{HH}$ = 8.0, 1H, C$H_{Ph,p}$), 7.08 – 7.02 (m, 9H, C$H_{PPh,o+p}$), 6.99 (d, 2H, $^{3}J_{HH}$ = 7.7 Hz, 1H, C$H_{Ph,o}$), 6.86 (d, $^{3}J_{HH}$ = 7.7 Hz, 1H, C$H_{Ph,o}$), 6.81 – 6.73 (m, 2H, C$H_{Ph,m}$), 1.42 (s, 18H, C$H_{3,tBu}$) ppm.
^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6): δ = 269.9 (s, CS_2), 180.6 (s, NCN), 134.1 (d, $^{3}J_{PC}$ = 10.2 Hz, $C_{PPh3,m}$), 132.6 (d, $^{4}J_{PC}$ = 3.1 Hz, $C_{PPh3,p}$), 130.6 (s, $C_{CPh,o}$), 129.5 (s, $C_{CPh,p}$), 128.9 (d, $^{2}J_{PC}$ = 12.5 Hz, $C_{PPh3,o}$), 128.5 (d, $^{2}J_{PC}$ = 12.4 Hz, CCN), 127.7 (d, $^{3}J_{PC}$ = 12.4 Hz, $C_{PPh3,m}$), 127.7 (s, $C_{Ph,m}$), 126.9 (d, $^{1}J_{PC}$ = 126.9 Hz, $C_{PPh3,ipso}$), 124.3 (s, $C_{CPh,ipso}$), 56.1 (s, $C(CH_3)_3$), 31.1 (s, C(CH_3)$_3$), 3.4 (d, $^{1}J_{PC}$ = 117.5 Hz, CCN) ppm.
^{29}Si{^{1}H}-NMR (79.5 MHz, C_6D_6): δ = -48.9 (d, $^{2}J_{Psi}$ = 22.0 Hz) ppm.
^{31}P{^{1}H}-NMR (162.0 MHz, C_6D_6): δ = 25.9 (s) ppm.

2.8 Synthesis of Silanone 6



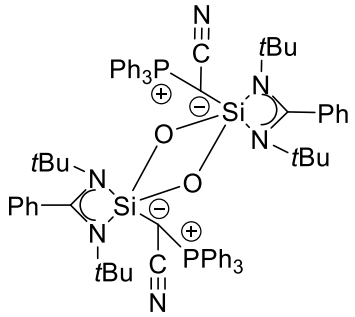
70.6 mg (0.10 mmol, 1 eq.) **AYSi-2** were added to a Schlenk tube and the atmosphere was exchanged to N_2O. The powder was stirred in that atmosphere overnight to yield the product as a colorless solid (65.4 mg, 0.09 mmol, 90%). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a saturated benzene solution of **6**.

^{1}H-NMR (400.3 MHz, C_4D_8O): δ = 8.10 (d, $^{3}J_{HH}$ = 7.9 Hz, 2H, C$H_{Tol,o}$), 7.61 – 7.54 (m, 2H, C$H_{Ph,o}$), 7.50 – 7.42 (m, 2H, C$H_{Ph,m}$), 7.41 – 7.33 (m, 1H, C$H_{Ph,p}$), 7.18 (d, $^{3}J_{HH}$ = 7.9 Hz, 2H C$H_{Tol,m}$), 3.54

– 3.38 (m, 3H, C$H_{Cy,ipso}$), 2.35 (s, 3H, C$H_{3,Tol}$), 1.92 – 1.78 (m, 6H, C$H_{Cy,m}$), 1.76 – 1.54 (m, 14H, C$H_{Cy,o+p}$), 1.36 – 1.08 (m, 28H, C$H_{Cy,m+p}$, C$H_{3,tBu}$) ppm.
$^{13}C\{^1H\}$-NMR (100.7 MHz, C_4D_8O): δ = 178.7 (s, N*C*N), 151.4 (s, $C_{Tol,ipso}$), 140.6 (s, $C_{Tol,p}$), 133.6 (s, $C_{Ph,ipso}$), 131.1 (s, $C_{Ph,o}$), 131.0 (s, $C_{Ph,o}$), 129.1 (s, $C_{Tol,m}$), 128.9 (s, $C_{Ph,m}$), 128.8 (s, $C_{Ph,m}$), 128.5 (s, $C_{Tol,p}$), 127.3 (s, $C_{Ph,o}$), 55.4 (s, $C(CH_3)_3$), 35.2 (d, $^1J_{PC}$ = 58.4 Hz, P*C*Si), 34.4 (d, $^1J_{PC}$ = 47.4 Hz, P$C_{Cy,ipso}$), 32.2 (s, C(CH_3)$_3$), 29.3 (d, $^3J_{PC}$ = 3.0 Hz, P$C_{Cy,m}$), 28.4 (d, $^2J_{PC}$ = 12.4 Hz, P$C_{Cy,o}$), 27.3 (s, P$C_{Cy,p}$), 21.4 (s, $CH_{3,Tol}$) ppm.
$^{29}Si\{^1H\}$-NMR (79.5 MHz, C_6D_6): δ = -40.6 (d, $^2J_{Psi}$ = 19.3 Hz) ppm.
$^{31}P\{^1H\}$-NMR (162.0 MHz, C_6D_6): δ = 32.3 (s) ppm.
Elem. Anal. Calcd. for $C_{41}H_{63}N_2O_3PSSi$: C, 68.10; H, 8.78; N, 3.87; S, 4.43. Found: C, 67.77; H, 8.39; N, 4.00; S, 4.15.

Alternative Synthesis of Silanone 6:
60.0 mg (84,9 µmol, 1 eq) **AYSi-2** were weight into a Schlenk flask and dissolved in 1.5 ml of toluene. The atmosphere was changed to 1.5 bar CO_2 and the solution was stirred for 1 d at RT. The next day the yellow solution had become a colorless suspension. The colorless precipitate was isolated by filtration and was washed with pentane (1.5 mL). The remaining colorless solid was identified as silanone **6** (22.1 mg, 30.6 µmol, 36 %).

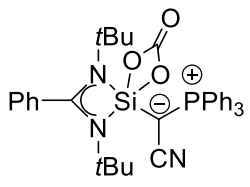
2.9 Synthesis of Siloxane 7



28 mg (0.05 mmol, 1 eq.) **AYSi-3** were dissolved in dry C_6D_6 in a J Young tube and the atmosphere was exchanged to 1 bar of N_2O. The reaction was stirred for one hour at room temperature and subsequently submitted for NMR experiments. Single crystals suitable for X-ray diffraction analysis formed during the reaction without stirring.

^{1}H-NMR (400.3 MHz, C_6D_6): δ = 8.15 – 8.04 (m, 8H, C$H_{PPh,o}$ + C$H_{CPh,o}$), 7.10 – 7.02 (m, 9H, C$H_{PPh3,m+p}$), 6.93 – 6.82 (m, 3H, C$H_{Ph,m+p}$), 1.31 (s, 18H, C(CH_3)$_3$) ppm.
$^{13}C\{^1H\}$-NMR (100.7 MHz, C_6D_6): δ = 175.84 (s, N*C*N), 134.57 (d, $^2J_{PC}$ = 10.2 Hz, $C_{PPh3,o}$), 132.17 (d, $^4J_{PC}$ = 2.9 Hz, $C_{PPh3,p}$), 131.41 (s, $C_{CPh,ipso}$), 129.32 (s, $C_{CPh,o}$), 129.27 (d, $^1J_{PC}$ = 18.7 Hz, $C_{PPh3,ipso}$), 128.72 (d, $^3J_{PC}$ = 12.4 Hz, $C_{PPh3,m}$), 127.68 (s, $C_{Ph,m}$), 126.92 (d, $^2J_{PC}$ = 2.7 Hz, C*C*N), 54.05 (s, *C*(CH_3)$_3$), 31.29 (s, C(CH_3)$_3$), 2.63 (d, $^1J_{PC}$ = 105.7 Hz, *C*CN) ppm.
$^{29}Si\{^1H\}$-NMR (79.5 MHz, C_6D_6): δ = -40.7 (d, $^2J_{Psi}$ = 18.2 Hz) ppm.
$^{31}P\{^1H\}$-NMR (162.0 MHz, C_6D_6): δ = 28.9 (s) ppm.

2.10 Synthesis of AYSi-2 carbonate complex 8

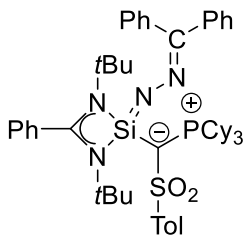


In a Schlenk flask, 60 mg (107 µmol, 1 eq) **AYSi-3** were dissolved in 2 ml toluene. The atmosphere was exchanged to 2 bar of CO_2 which led within minutes to a color change of the solution from orange to violet. After further stirring for 1 d at RT the solution had turned into a colorless suspension. The colorless precipitate was isolated from the supernatant solution. The residue

was dried *in vacuo* to yield the product as a white solid (25.8 mg, 41.6 µmol, 39%). Crystals suitable for XRD were won by slow vapor diffusion of hexane into a saturated solution of **8** in benzene.

^{1}H-NMR (400 MHz, C_6D_6) δ = 7.92 (ddd, $^{3}J_{PH}$ = 12.4, $^{3}J_{HH}$ = 7.4, $^{4}J_{HH}$ = 2.1 Hz, 6H, C$H_{PPh,o}$), 7.72 (d, $^{3}J_{HH}$ = 7.6 Hz, 1H, C$H_{Ph,p}$), 7.08 (m, 9H, C$H_{PPh,m}$ + C$H_{PPh,p}$), 6.85 (m, 4H, C$H_{Ph,o+p}$), 1.22 (s, 18H, C$H_{3,t\mathrm{Bu}}$) ppm.
^{13}C{^{1}H}-NMR (101 MHz, C_6D_6) δ = 176.3 (N*C*N), 153.1 (O(*C*O)O), 133.5 (d, $^{2}J_{PC}$ = 9.5 Hz, *C*H$_{PPh,o}$), 132.2 (d, $^{4}J_{PC}$ = 2.9 Hz, *C*H$_{PPh,p}$), 132.1 (*C*H$_{CPh,ipso}$), 130.3 (*C*H$_{CPh,p}$), 130.1 (*C*H$_{Ph,m}$), 129.1 (d, $^{3}J_{PC}$ = 12.1 Hz, *C*H$_{PPh,m}$), 127.7 (*C*H$_{CPh,o}$), 126.5 (*C*H$_{PPh,ipso}$), 54.6 (*C*(CH$_3$)$_{3,t\mathrm{Bu}}$), 31.1 (C(*C*H$_3$)$_{3,t\mathrm{Bu}}$), 2.4 (d, $^{1}J_{PH}$ = 101.1 Hz, *C*CN) ppm.
^{29}Si{^{1}H}-NMR (80 MHz, C_6D_6) δ = -90.2 (d, $^{2}J_{PSi}$ = 18.0 Hz) ppm.
^{31}P{^{1}H}-NMR (162 MHz, C_6D_6) δ = 28.2 ppm.

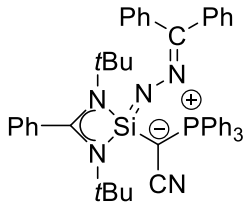
2.10 Synthesis of Silazine 9_{Ts}



70.6 mg (0.10 mmol, 1 eq.) **AYSi-2** and 19.4 mg (0.10 mmol, 1 eq.) 1,1'-diphenyl diazomethane were dissolved in 3 ml toluene and the reaction was stirred overnight at room temperature. The reaction mixture was filtered, and the precipitate was washed with 3 ml cold toluene and subsequently dried *in vacuo*. The precipitate was recrystallized by slow vapor diffusion of hexane into a saturated solution of **9_{Ts}** in THF. The supernatant solution was taken off and the crystals were dried *in vacuo* to obtain the product as a yellow solid (50.3 mg, 0.06 mmol, 62%). After recrystallization, a few crystals were taken for X-ray diffraction analysis.

^{1}H-NMR (400.3 MHz, C_4D_8O): δ = 8.07 (d, $^{3}J_{HH}$ = 7.9 Hz, 2H, C$H_{Tol,o}$), 7.76 (d, $^{3}J_{HH}$ = 7.4 Hz, 1H, C$H_{Ph,o}$), 7.63 (d, $^{3}J_{HH}$ = 7.4 Hz, 1H, C$H_{Ph,o}$), 7.57 – 7.47 (m, 4H, C$H_{Ph2,o}$), 7.42 (t, $^{3}J_{HH}$ = 7.4 Hz, 1H C$H_{Ph,p}$), 7.34 – 7.27 (m, 4H, C$H_{Ph2,m}$), 7.23 (d, $^{3}J_{HH}$ = 7.9 Hz, C$H_{Tol,m}$), 7.18 – 7.12 (m, 1H, C$H_{Ph,o}$), 7.08 (d, $^{3}J_{HH}$ = 7.4 Hz, 2H, C$H_{Ph2,p}$), 6.95 – 6.87 (m, 1H, C$H_{Ph,m}$), 3.24 – 3.10 (m, 3H, C$H_{Cy,ipso}$), 2.36 (s, 3H, C$H_{3,Tol}$), 1.82 – 1.66 (m, 12H, C$H_{Cy,o}$), 1.64 – 1.53 (m, 6H, C$H_{Cy,m}$), 1.49 – 1.38 (m, 6H, C$H_{Cy,p}$), 1.32 (s, 18H, C$H_{3,t\mathrm{Bu}}$), 1.11 – 1.04 (m, 6H, C$H_{Cy,m}$) ppm.
^{13}C{^{1}H}-NMR (100.7 MHz, C_4D_8O): δ = 178.0 (s, N*C*N), 150.5 (s, *C*$_{Tol,ipso}$), 146.5 (s, *C*$_{N2}$), 144.4 (s, *C*$_{Ph2,ipso}$), 142.9 (s, *C*$_{Ph2,ipso}$), 141.1 (s, *C*$_{Tol,p}$), 133.1 (s, *C*$_{Ph,ipso}$), 132.1 (s, *C*$_{Ph2,o}$), 131.2 (s, *C*$_{Ph,m}$), 131.0 (s, *C*$_{Ph,o}$), 129.6 (s, *C*$_{Ph,o}$), 129.3 (s, *C*$_{Tol,m}$), 128.8 (s, *C*$_{Ph,p}$), 128.5 (s, *C*$_{Ph2,o}$), 128.4 (s, *C*$_{Ph2,m}$), 128.0 (s, *C*$_{Ph2,m}$), 127.4 (s, *C*$_{Tol,o}$), 126.4 (s, *C*$_{Ph2,p}$), 125.8 (s, *C*$_{Ph2,o}$), 124.5 (s, *C*$_{Ph2,p}$), 55.3 (s, *C*(CH$_3$)$_3$), 35.0 (d, $^{1}J_{PC}$ = 47.4 Hz, P*C*$_{Cy,ipso}$), 34.6 (d, $^{1}J_{PC}$ = 58.4 Hz, P*C*Si), 32.2 (s, C(*C*H$_3$)$_3$), 29.3 (s, P*C*$_{Cy,m}$), 28.0 (d, $^{2}J_{PC}$ = 12.3 Hz, P*C*$_{Cy,o}$), 27.0 (s, P*C*$_{Cy,p}$), 21.4 (s, *C*H$_{3,Tol}$) ppm.
^{29}Si{^{1}H}-NMR (79.5 MHz, C_6D_6): δ = -16.5 ppm. (A coupling constant was not determined since the shift was determined by ^{1}H-^{29}Si-HMBC experiments.)
^{31}P{^{1}H}-NMR (162.0 MHz, C_6D_6): δ = 31.5 (s) ppm.

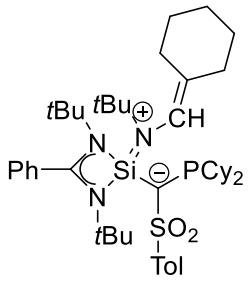
2.11 Synthesis of Silazine $\mathbf{9_{CN}}$



54.9 mg (98.1 µmol, 1 eq) **AYSi-3** were dissolved in 1 ml benzene and a solution of 20.0 mg (103 µmol, 1.05 eq) 1,1'-diphenyl diazomethane in 0.5 ml benzene was added. The orange solution was stirred for 1 d at RT and subsequently overlayered with 3 ml pentane. Within minutes yellow crystals formed. After 1 d the supernatant solution was removed from the yellow solid, which were washed once with 3 ml pentane. The remaining yellow solid (48.1 mg, 63.8 µmol, 65 %) was characterized as the targeted product. Crystals suitable for XRD were won by slow vapor diffusion of hexane into a saturated solution of $\mathbf{9_{CN}}$ in THF.

^{1}H-NMR (400 MHz, THF-d$_8$) δ = 7.74 (m, 6H, C$H_{PPh,o}$), 7.62 (m, 1H, C$H_{PhCPh,p}$), 7.55 (ddt, $^3J_{HH}$ = 7.0, $^4J_{HH}$ = 3.6, $^5J_{PH}$ = 1.4 Hz, 3H, C$H_{PPh,p}$), 7.50 (m, 5H, C$H_{PhCPh,o}$ + C$H_{PhCPh,p}$), 7.36 (td, J = 7.9, 3.2 Hz, 6H, C$H_{PPh,m}$), 7.07 (m, 4H, C$H_{PhCPh,m}$), 7.00 (m, 4H, C$H_{CPh,o}$ + C$H_{CPh,m}$), 6.93 (m, 1H, C$H_{CPh,p}$), 1.13 (s, 18H, C$H_{3,t\mathrm{Bu}}$) ppm.
^{13}C{^{1}H}-NMR (101 MHz, THF-d$_8$) δ = 177.9 (N*C*N), 147.7 (*C*$_{PhCPh,ipso}$), 144.2 (Ph*C*Ph), 140.4 (*C*$_{CPh,ipso}$), 135.2 (d, $^2J_{PC}$ = 10.3 Hz, *C*$_{PPh,o}$), 132.8 (d, $^4J_{PC}$ = 3.0 Hz, *C*$_{PPh,p}$), 131.7 (*C*$_{PhCPh,m}$), 130.1 (d, $^1J_{PC}$ = 382.6 Hz, *C*$_{PPh,ipso}$), 129.1 (d, $^3J_{PC}$ =12.8 Hz, *C*$_{PPh,m}$), 129.0 (*C*$_{PhCPh,p}$), 128.0 (*C*$_{PhCPh,o}$) 127.9 (*C*$_{CPh,m}$), 126.3 (*C*$_{PhCPh,p}$), 125.9 (*C*$_{CPh,o}$), 125.2 (d, $^2J_{PC}$ = 2.1 Hz, C*C*N), 124.9 (*C*$_{CPh,p}$), 54.9 (*C*(CH$_3$)$_{3,t\mathrm{Bu}}$), 31.3 (C(*C*H$_3$)$_{3,t\mathrm{Bu}}$).
^{31}P{^{1}H}-NMR (162 MHz, THF-d$_8$) δ = 26.6 ppm.
HRMS-LIFDI (m/z): [M]$^+$ calcd for $C_{48}H_{48}N_5PSi$, 753.3417; found, 753.3401.

2.12 Synthesis of 10



70.6 mg (0.10 mmol, 1 eq.) **AYSi-2** was dissolved in 3 ml toluene and 11.6 µL (0.10 mmol, 1 eq.) *tert*-butyl isocyanide were added. The reaction was heated to 40 °C overnight. After cooling to room temperature, the volatiles were removed *in vacuo* and 5 ml acetonitrile were added to the residue. A white precipitate formed which was filtered and washed with 2 ml of cold pentane. The residue was dried *in vacuo* to yield the product as a white solid (56.9 mg, 0.07 mmol, 72%). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a saturated pentane solution of **10**.

^{1}H-NMR (400.3 MHz, C_6D_6): δ = 8.40 (d, $^3J_{HH}$ = 8.3 Hz, 2H, C$H_{Tol,o}$), 7.76 (t, $^3J_{HH}$ = 7.0 Hz, 1H, C$H_{Ph,o}$), 7.18 – 7.15 (m, 1H, C$H_{Ph,o}$), 7.03 (m, $^3J_{HH}$ = 8.3 Hz, 2H, C$H_{Tol,m}$), 6.98 – 6.88 (m, 4H, C$H_{Ph,o+m+p}$), 6.32 (s, 1H, NC*H*), 2.57 – 2.41 (m, 4H, NC$H_{Cy,o}$), 2.39 – 2.29 (m, 4H, PC$H_{Cy,o}$), 2.25 – 2.17 (m, 2H, PC$H_{Cy,ipso}$), 2.06 (s, 3H, C$H_{3,Tol}$), 1.92 – 1.74 (m, 8H, PC$H_{Cy,m}$), 1.71 (s, 9H, NC$H_{3,t\mathrm{Bu}}$), 1.64 – 1.52 (m, 6H, NC$H_{Cy,p}$ + PC$H_{Cy,p}$), 1.45 (s, 18H, C$H_{3,t\mathrm{Bu}}$), 1.39 – 1.29 (m, 4H, NC$H_{Cy,m}$) ppm.
^{13}C{^{1}H}-NMR (100.7 MHz, C_6D_6): δ = 176.5 (s, N*C*N), 148.9 (s, *C*$_{Tol,p}$), 140.0 (s, *C*$_{Tol,ipso}$), 138.7 (s, NC*C*$_{Cy}$), 131.8 (s, *C*$_{Ph,ipso}$), 130.4 (s, *C*$_{Ph,o}$), 129.5 (s, *C*$_{Tol,m}$), 129.4 (s, *C*$_{Ph,p}$), 128.6 (s, *C*$_{Tol,o}$), 127.7 (s, *C*$_{Ph,m}$), 127.1 (s, N*C*C$_{Cy}$), 57.9 (s, N*C*(CH$_3$)$_3$), 55.7 (s, *C*(CH$_3$)$_3$), 47.8 (d, $^1J_{PC}$ = 62.3z Hz, P*C*Si), 36.1 (d, $^2J_{PC}$ = 14.7 Hz, P*C*$_{Cy,o}$), 35.0 (s, NC*C*$_{Cy,o}$), 33.9 (d, $^1J_{PC}$ = 19.4 Hz, P*C*$_{Cy,ipso}$), 32.4 (d, $^2J_{PC}$ = 14.5 Hz, P*C*$_{Cy,o}$), 32.3 (s, C(*C*H$_3$)$_3$), 30.5 (s, NC(*C*H$_3$)$_3$), 30.3 (s, NC*C*$_{Cy,o}$), 28.5 (s, P*C*$_{Cy,p}$),

28.3 (d, $^{3}J_{PC}$ = 9.1 Hz, P$C_{Cy,m}$), 28.2 (s, NC$C_{Cy,m}$), 27.5 (s, P$C_{Cy,p}$), 27.3 (s, NC$C_{Cy,m}$), 26.7 (s, NC$C_{Cy,m}$), 21.2 (s, CH$_{3,Tol}$) ppm.
^{29}Si{^{1}H}-NMR (79.5 MHz, C_6D_6): δ = -42.1 ppm. (A coupling constant was not determined since the shift was determined by ^{1}H-^{29}Si-HMBC experiments.)
^{31}P{^{1}H}-NMR (162.0 MHz, C_6D_6): δ = -13.9 (s) ppm.
HRMS-LIFDI (m/z): $[M]^+$ calcd for $C_{46}H_{72}N_3O_2PSSi$, 789.4852; found, 789.4836.

3 Stability test monitored by NMR spectroscopy

3.1 Stability of silylene AYSi-2 in toluene

Procedure for stability testing: **AYSi-2** (20 mg) was dissolved in 0.6 mL toluene inside a J-Young NMR tube, which was heated to 50 °C over a period of 2 weeks. To represent the progress of decomposition, the ^{31}P NMR spectra measured before the heating, after 1 d, after 5 d, after 1 week and after 2 weeks are depicted.

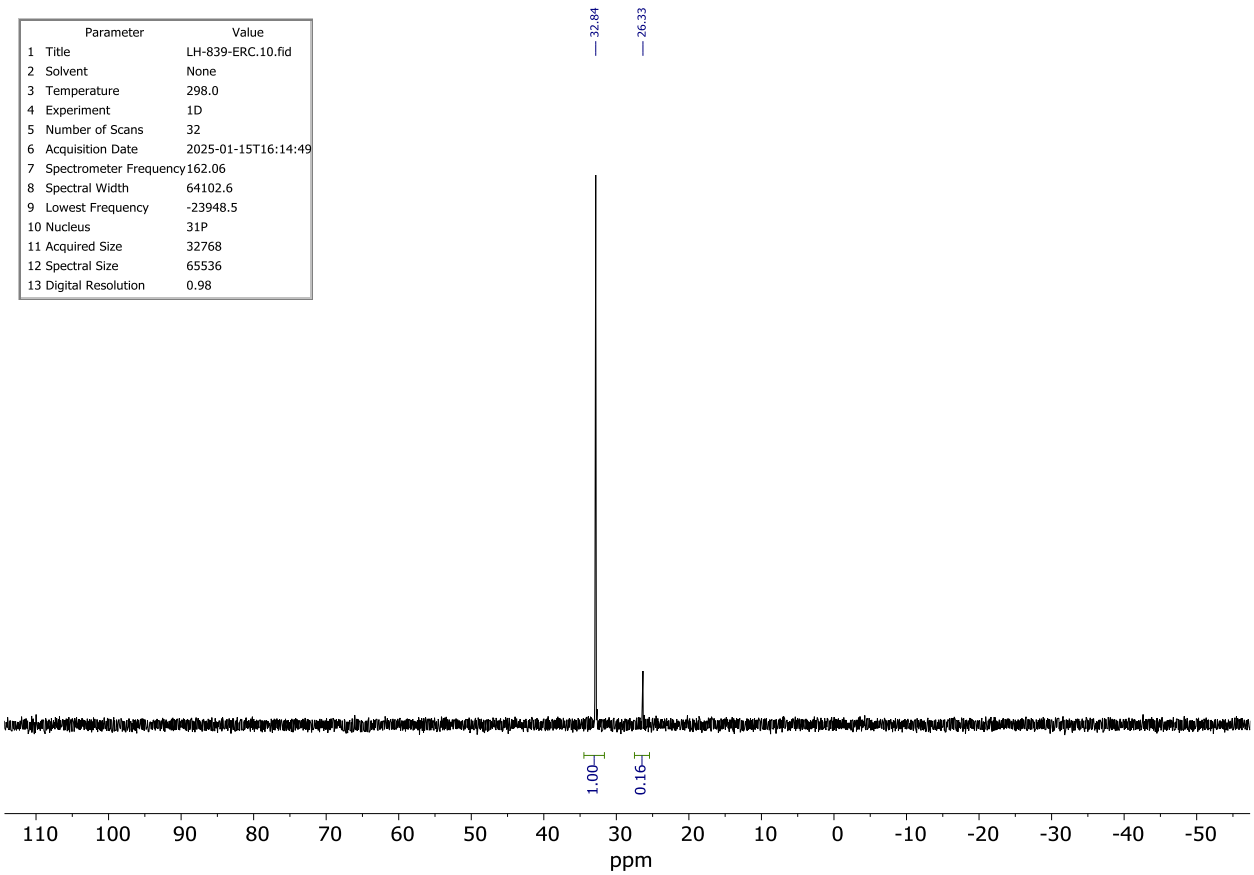


Figure S1. $^{31}P\{^{1}H\}$-NMR spectrum of **AYSi-2** measured in toluene before heating.

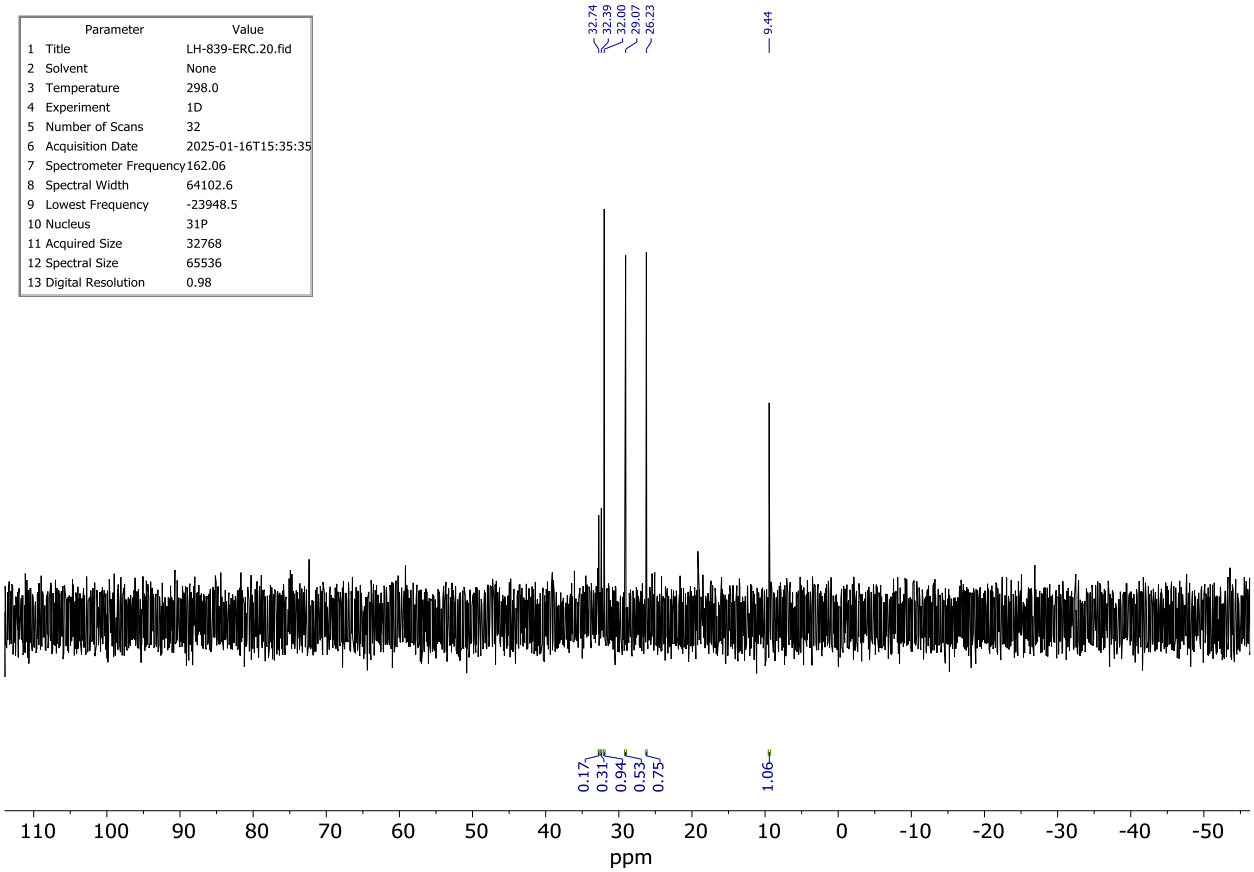


Figure S2. $^{31}P\{^{1}H\}$-NMR spectrum measured in toluene after heating **AYSi-2** to 50 °C for 1 d.

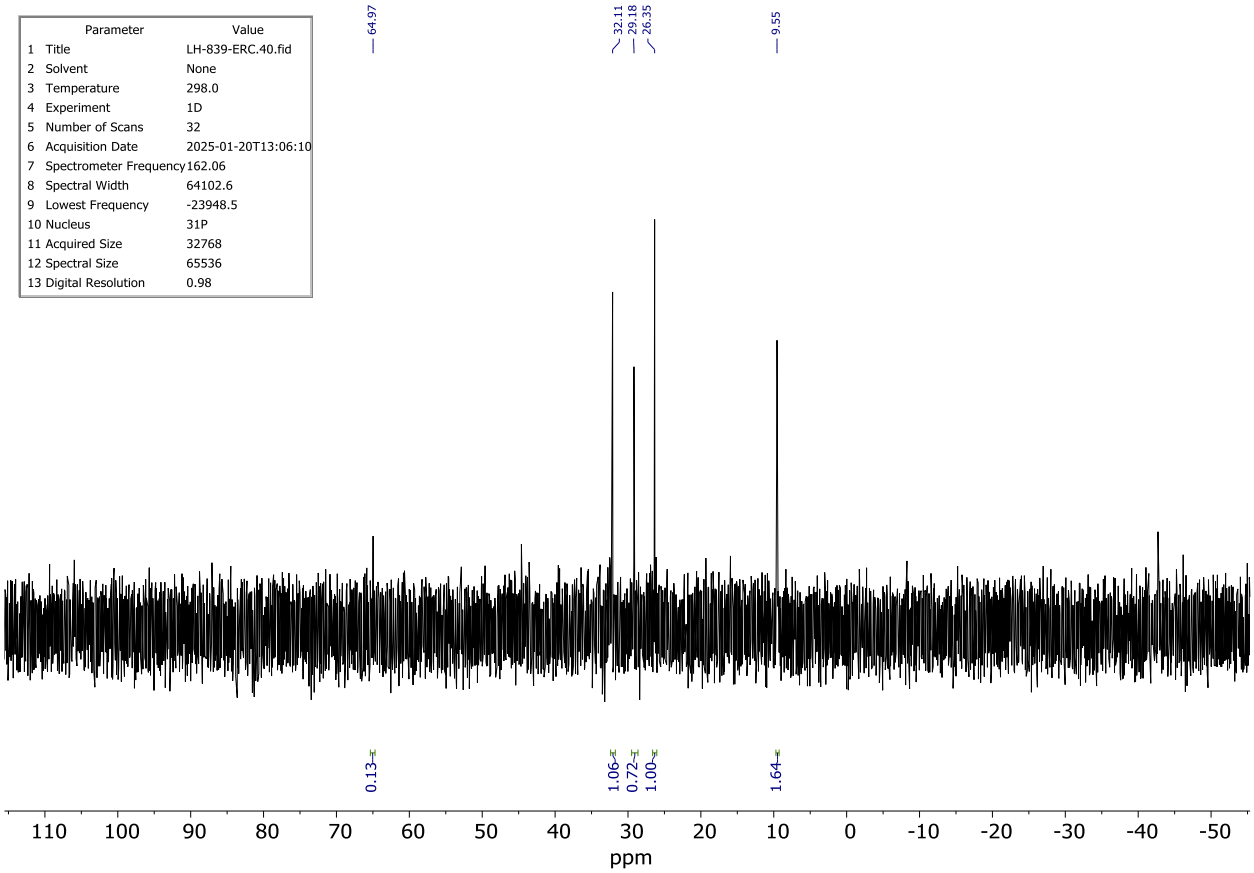


Figure S3. $^{31}P\{^{1}H\}$-NMR spectrum measured in toluene after heating **AYSi-2** to 50 °C for 5 d.

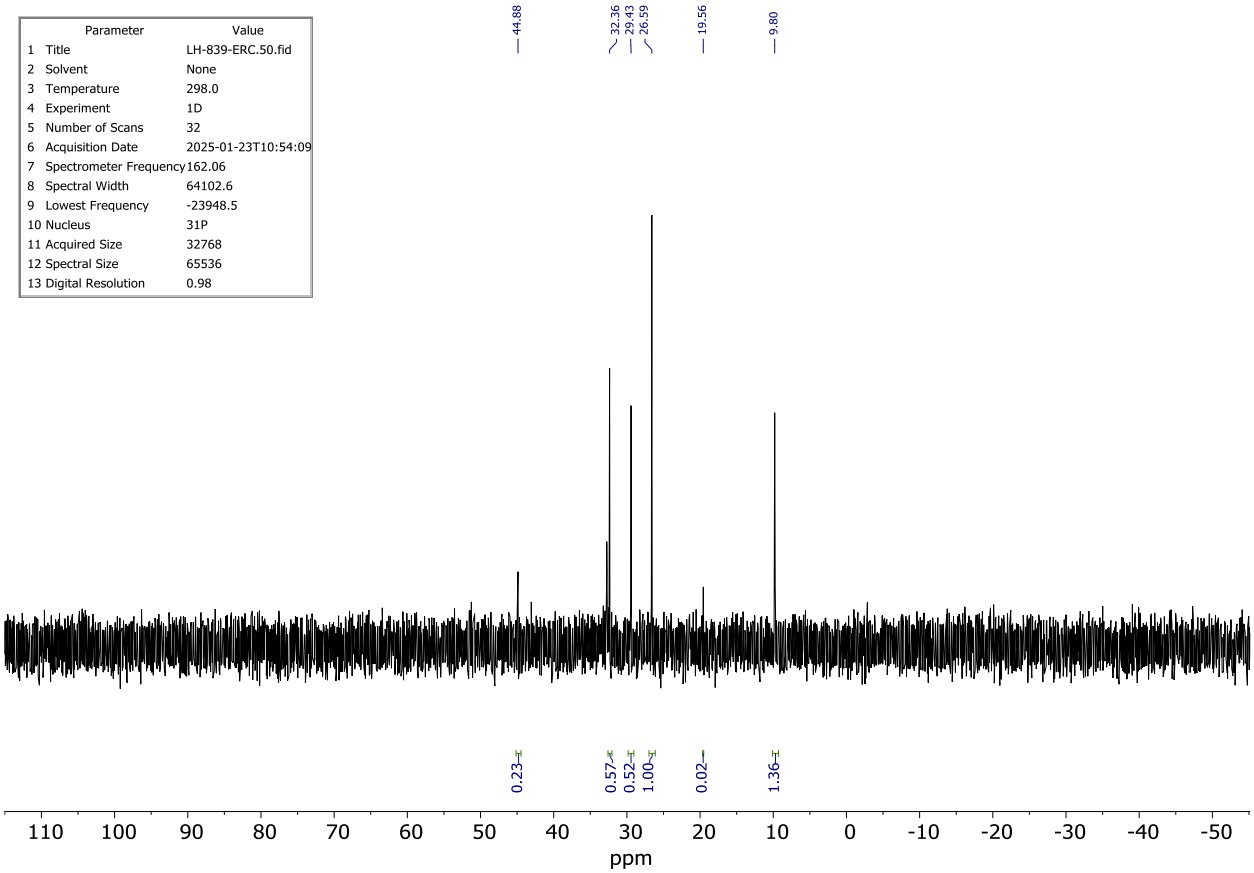


Figure S4. $^{31}P\{^{1}H\}$-NMR spectrum measured in toluene after heating **AYSi-2** to 50 °C for 1 week.

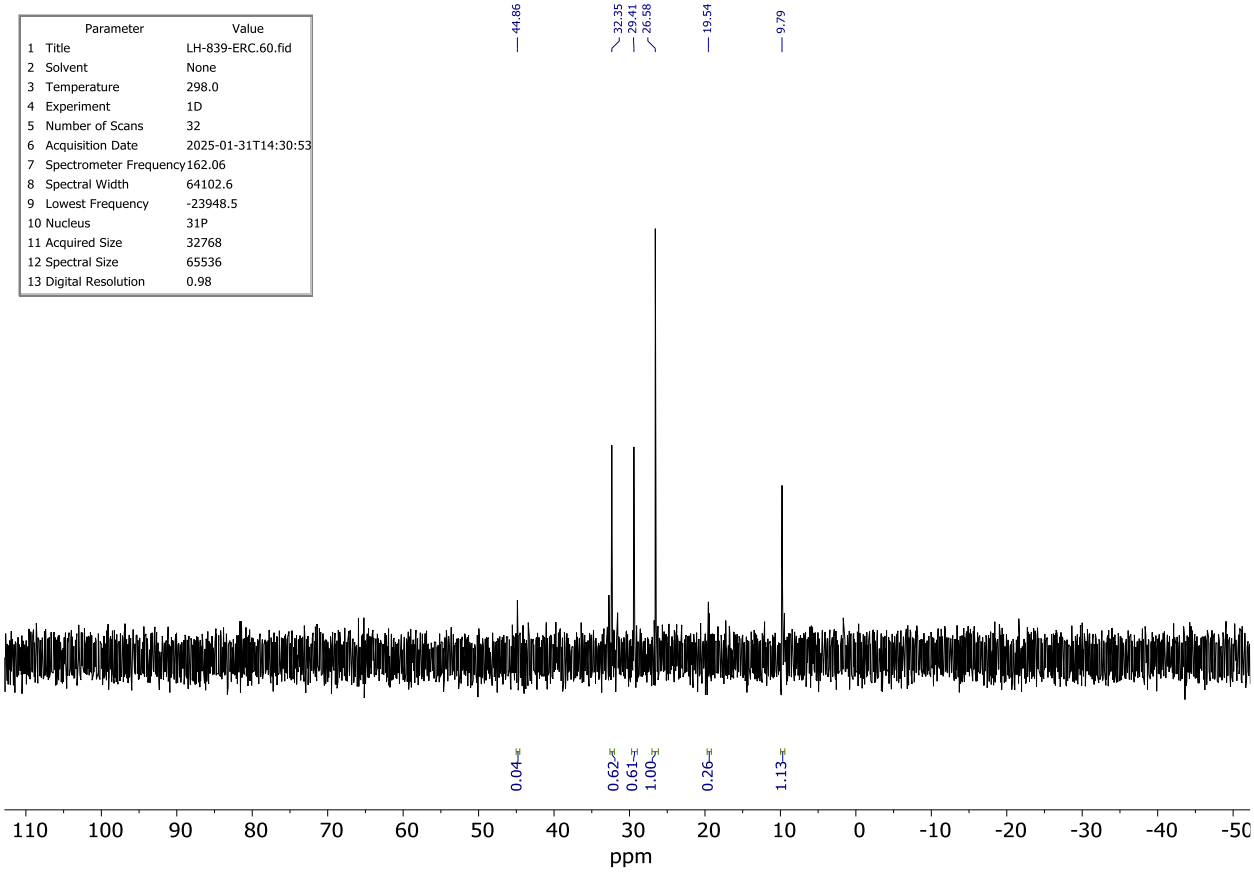


Figure S5. $^{31}P\{^{1}H\}$-NMR spectrum measured in toluene after heating **AYSi-2** to 50 °C for 2 weeks.

3.2 stability of silylene AYSi-3 in C_6D_6

Procedure for stability testing: **AYSi-2** (40 mg) was dissolved in 0.6 mL C_6D_6 in a J-Young NMR tube. The mixture was heated to 70 °C over a period of 4d. To follow the conversion to the C-H activation product, ^{31}P NMR spectra were measured after 1 d and after 4 d of heating. The spectra a presented below. To identify the formed product, a ^{1}H-NMR spectrum was recorded after 4 d of heating. As shown in Figure S8, the spectrum clearly indicates the formation of a Si-H moiety, with the proton appearing at 6.32 ppm featuring additional ^{29}Si satellites.

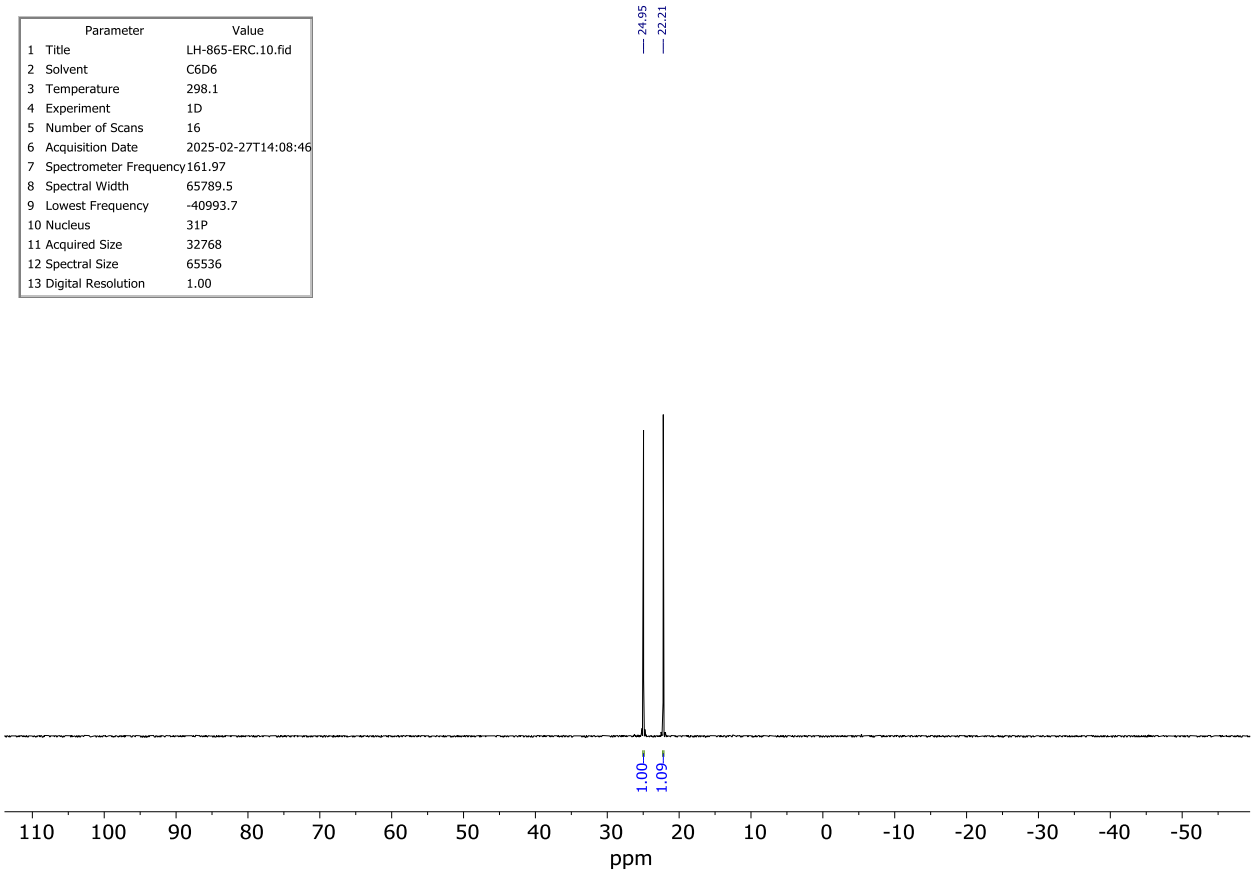


Figure S6. $^{31}P\{^{1}H\}$-NMR spectrum measured in C_6D_6 after heating **AYSi-3** to 70 °C for 1 d.

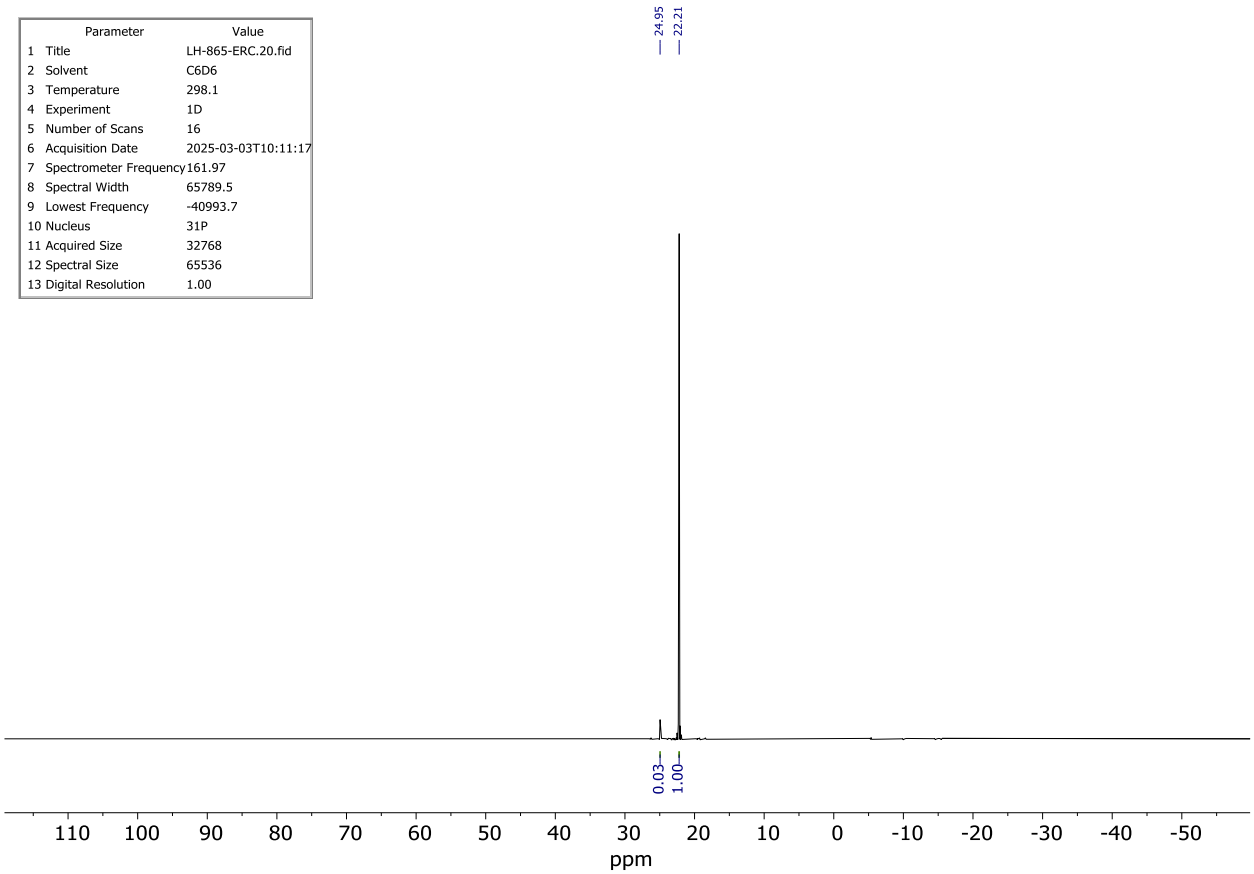


Figure S7. $^{31}P\{^{1}H\}$-NMR spectrum measured in C_6D_6 after heating **AYSi-3** to 70 °C for 4 d.

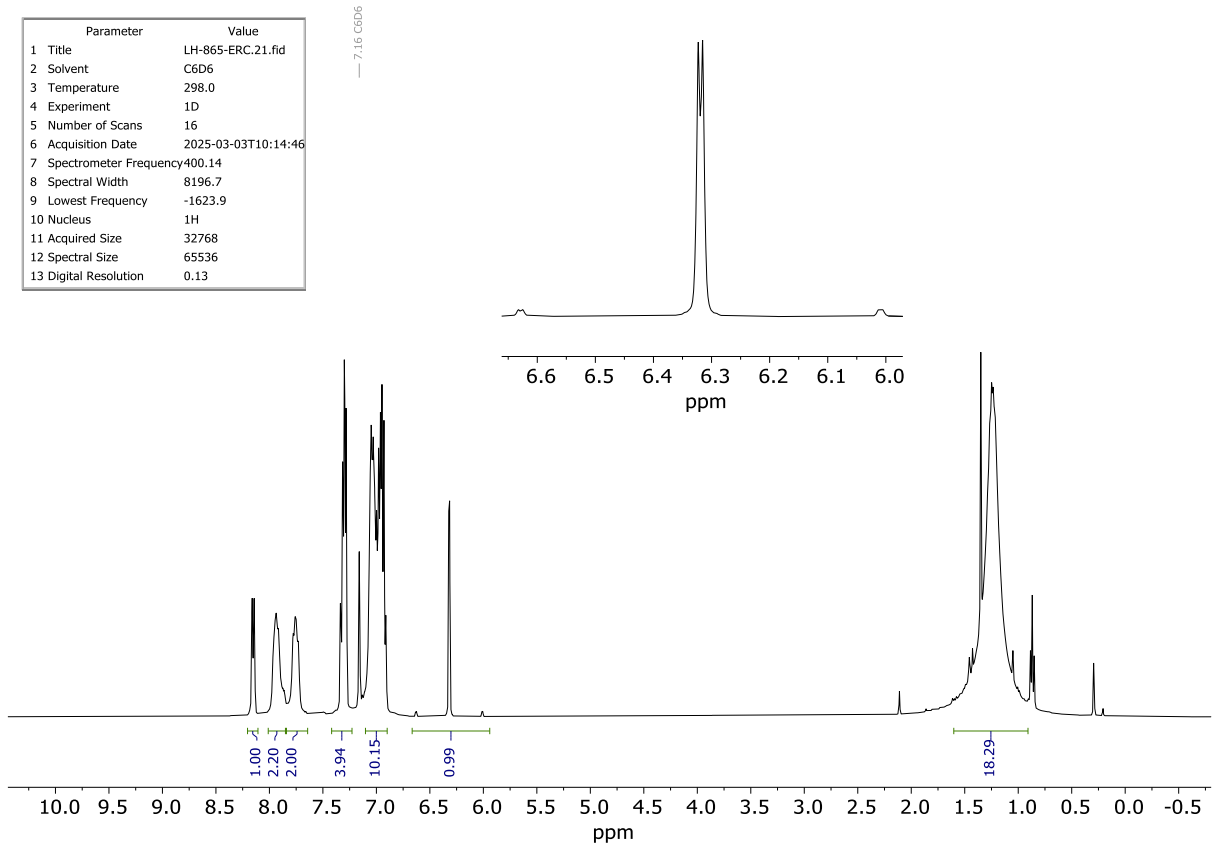


Figure S8. ^{1}H-NMR spectrum measured in C_6D_6 after heating **AYSi-3** to 70 °C for 4 d. The doublet at 6.32 ppm was identified as the Si-H signal due to the display of ^{29}Si-satellites, highlighted in the expansion of the spectrum.

3.3 Stability of silanone 6 in THF

Procedure for stability testing: A fresh batch of **6** was prepared by the exposure of solid **AYSi-2** to 1 bar of N_2O. The solid was taken up in dry THF-d_8 and added to an oven-dried J-Young tube. The freshly prepared sample already showed some ylide impurities (26.59 ppm) which was used as reference in the further studies. Fort stability test, the sample was kept in THF at room temperature and NMR spectra were recorded after 5 days, 1 month and 2 months.

Additionally, VT ^{1}H-NMR experiments were performed at 60 °C and -30 °C to investigate the interaction of the Cy-H *ipso*-protons with the oxygen atom at the silicon atom. While heating to 60 °C led to an improved resolution of the corresponding multiplett at 6.37 ppm, arguing for increased coalescence, cooling to –30 °C led to complete disappearance of the signal. This further corroborates with a weak interaction of the C-H moiety with the silanone.

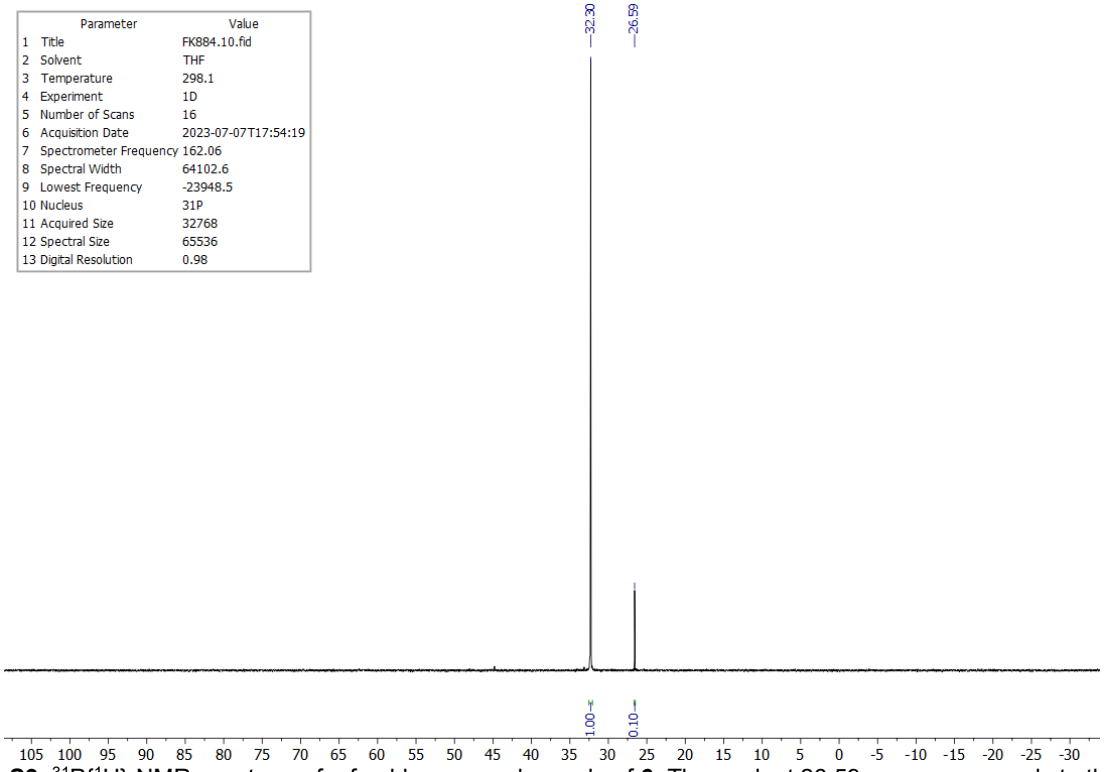


Figure S9. ^{31}P{^{1}H}-NMR spectrum of a freshly prepared sample of **6**. The peak at 26.59 ppm corresponds to the ylide which serves as an internal standard.

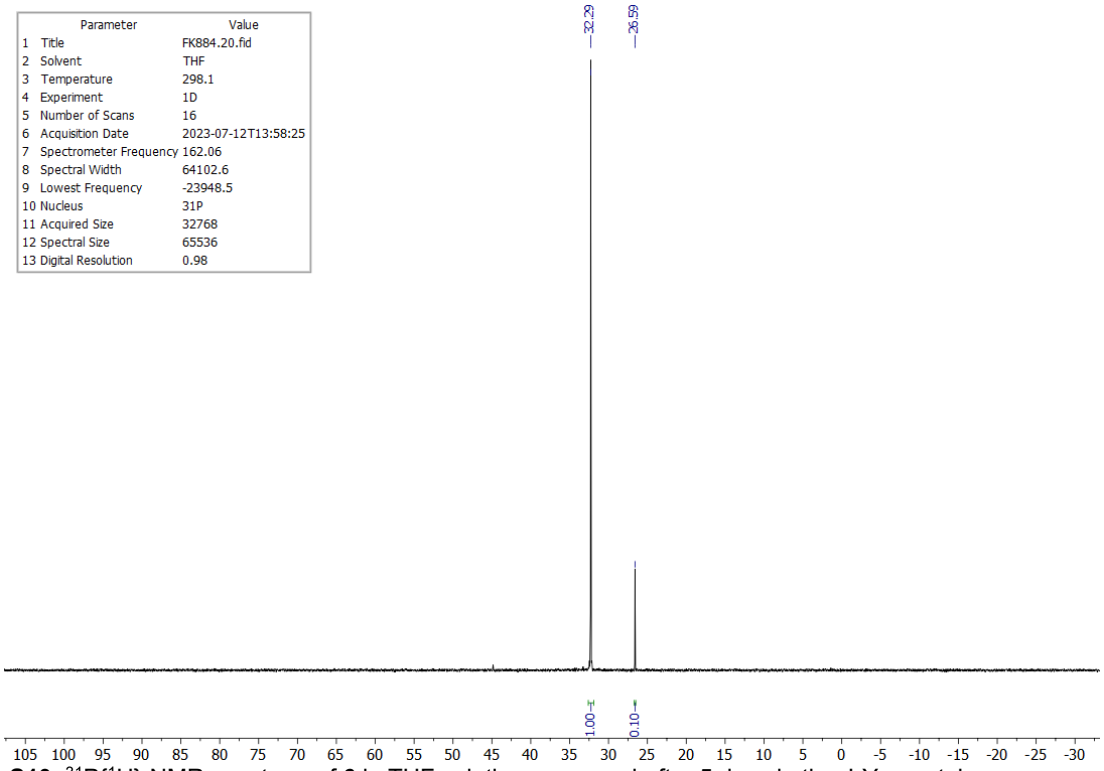


Figure S10. $^{31}P\{^{1}H\}$-NMR spectrum of **6** in THF solution measured after 5 days in the J-Young tube.

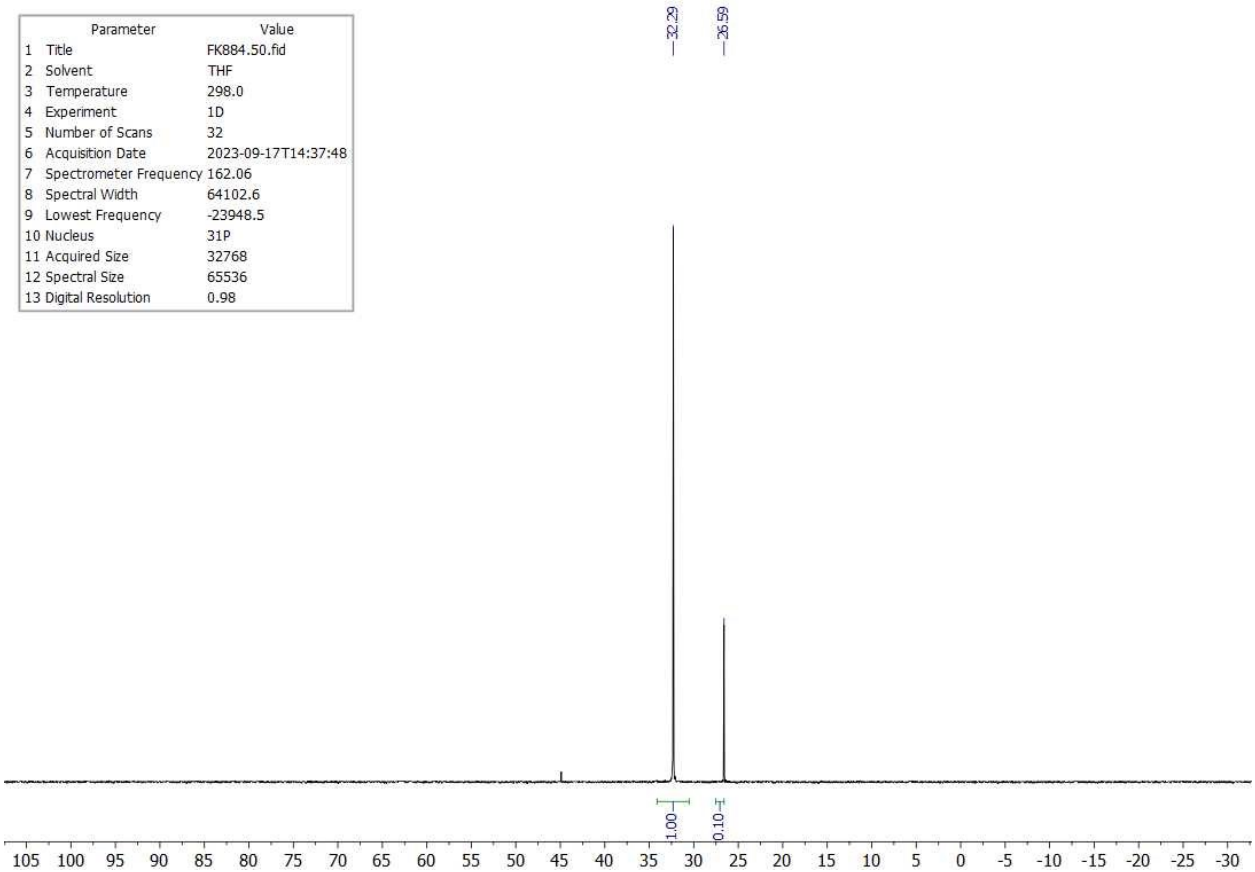


Figure S11. $^{31}P\{^{1}H\}$-NMR spectrum of **6** in THF solution measured after 2 months in the J-Young tube.

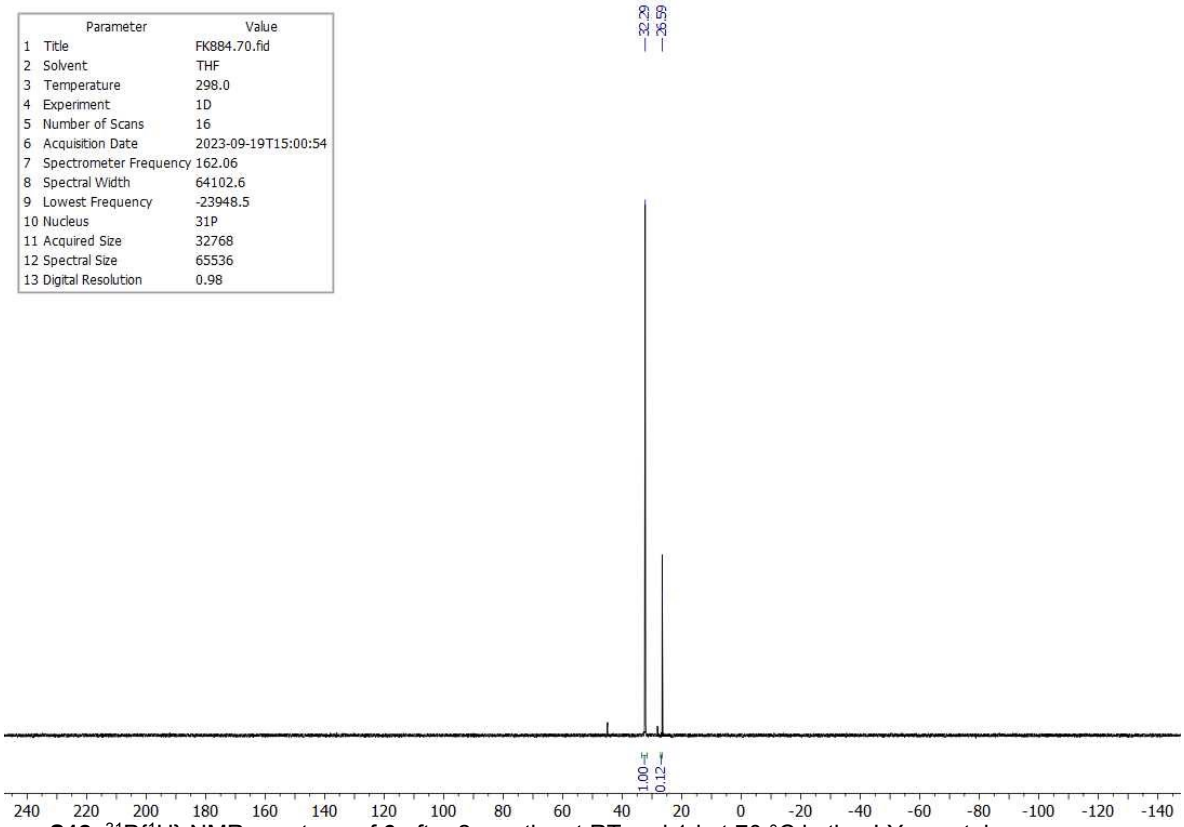


Figure S12. $^{31}P\{^{1}H\}$-NMR spectrum of **6** after 2 months at RT and 1d at 70 °C in the J-Young tube.

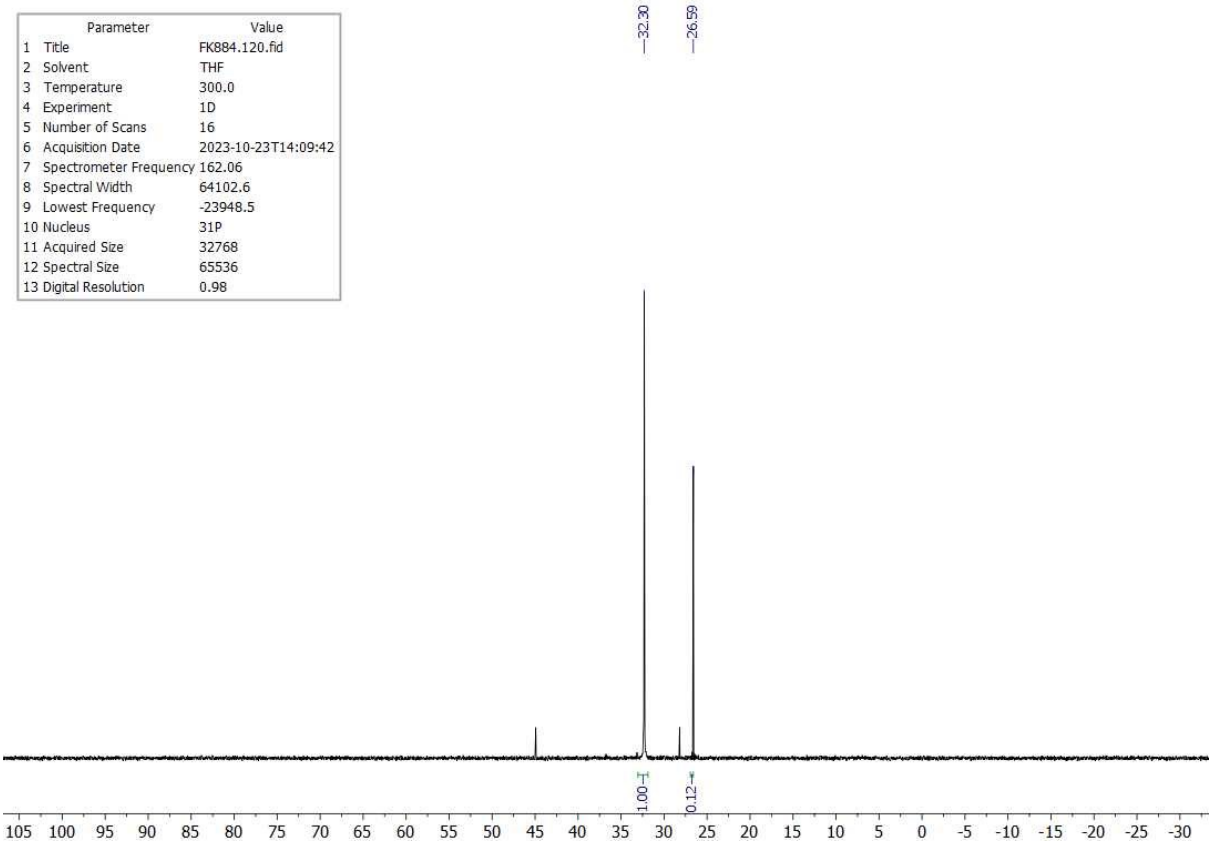


Figure S13. $^{31}P\{^{1}H\}$-NMR spectrum of **6** after 2 months at RT and 1 month at 70 °C in the J-Young tube.

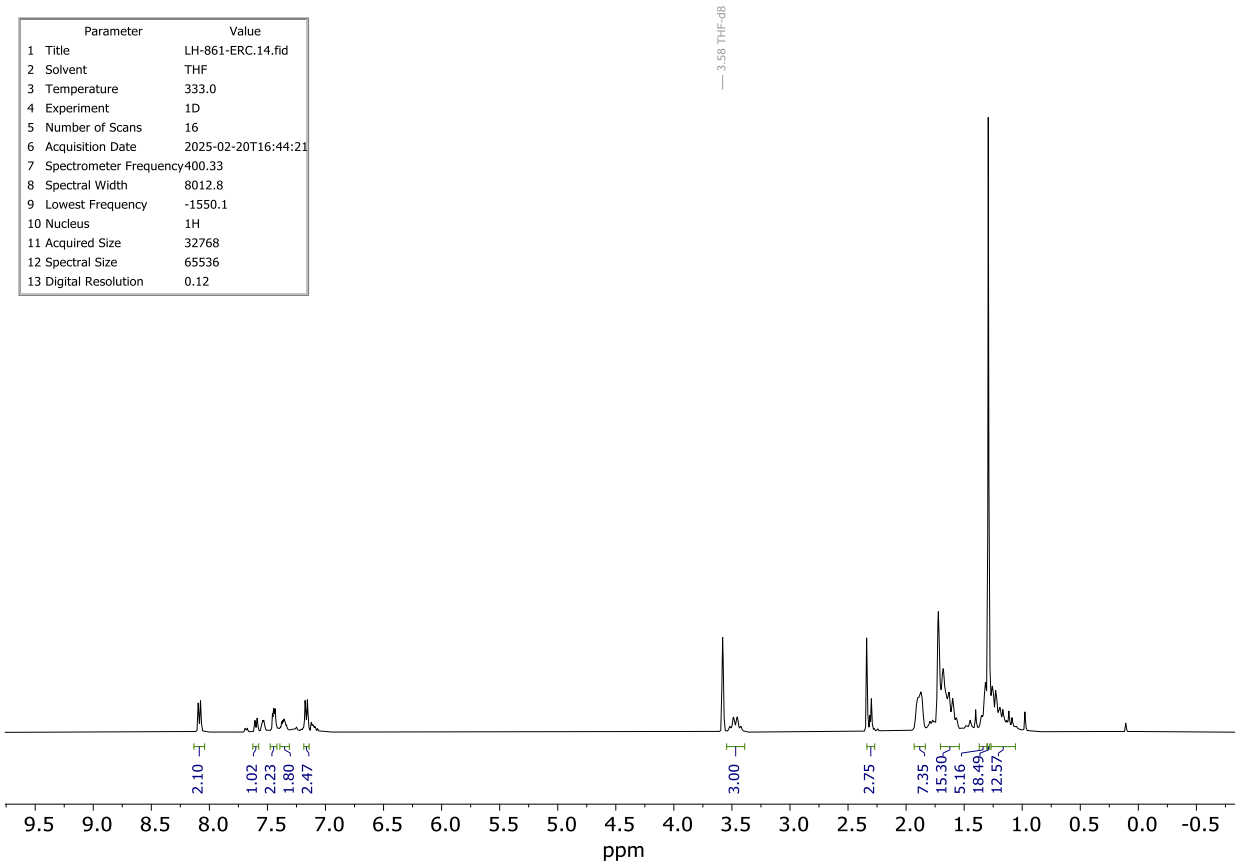


Figure S14. ^{1}H-NMR spectrum of **6** measured in d_8-THF at 333K.

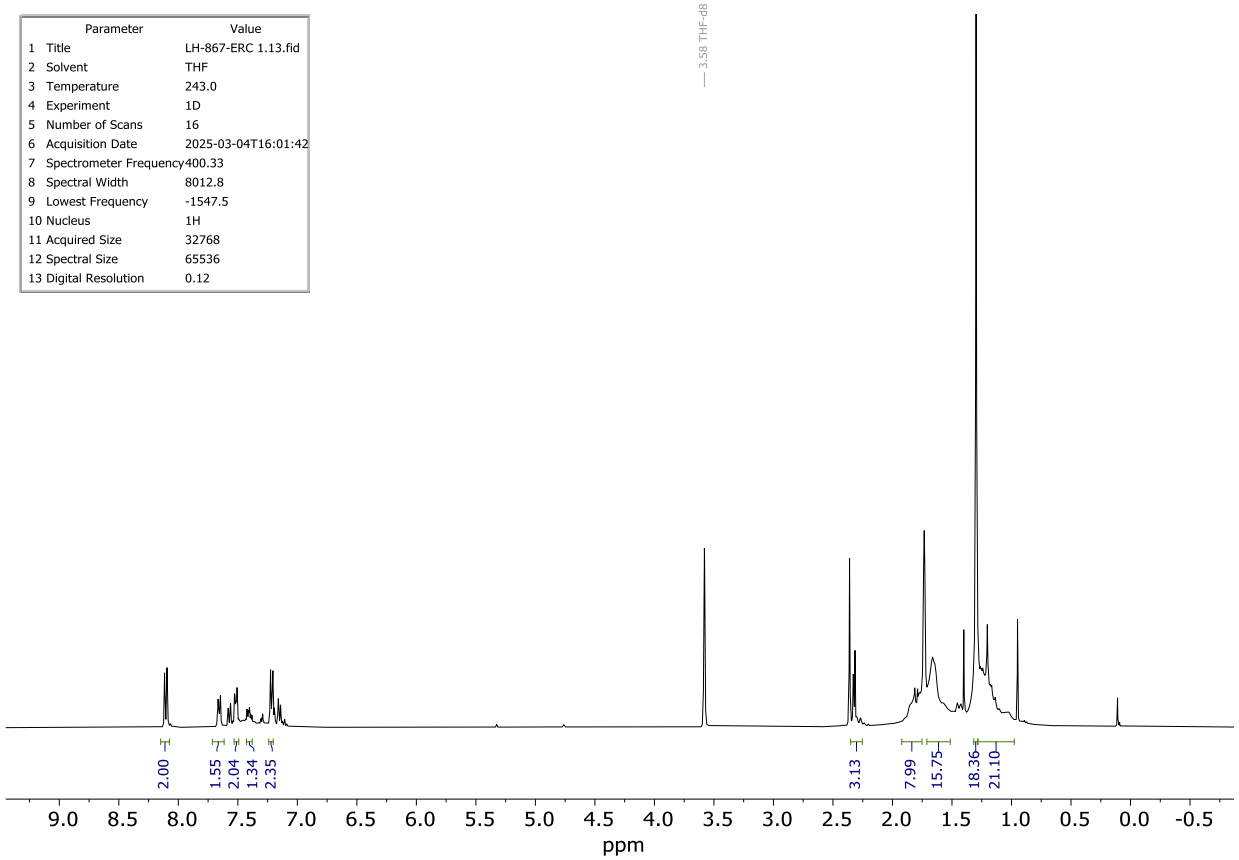


Figure S15. ^{1}H-NMR spectrum of **6** measured in d_8-THF at 243K.

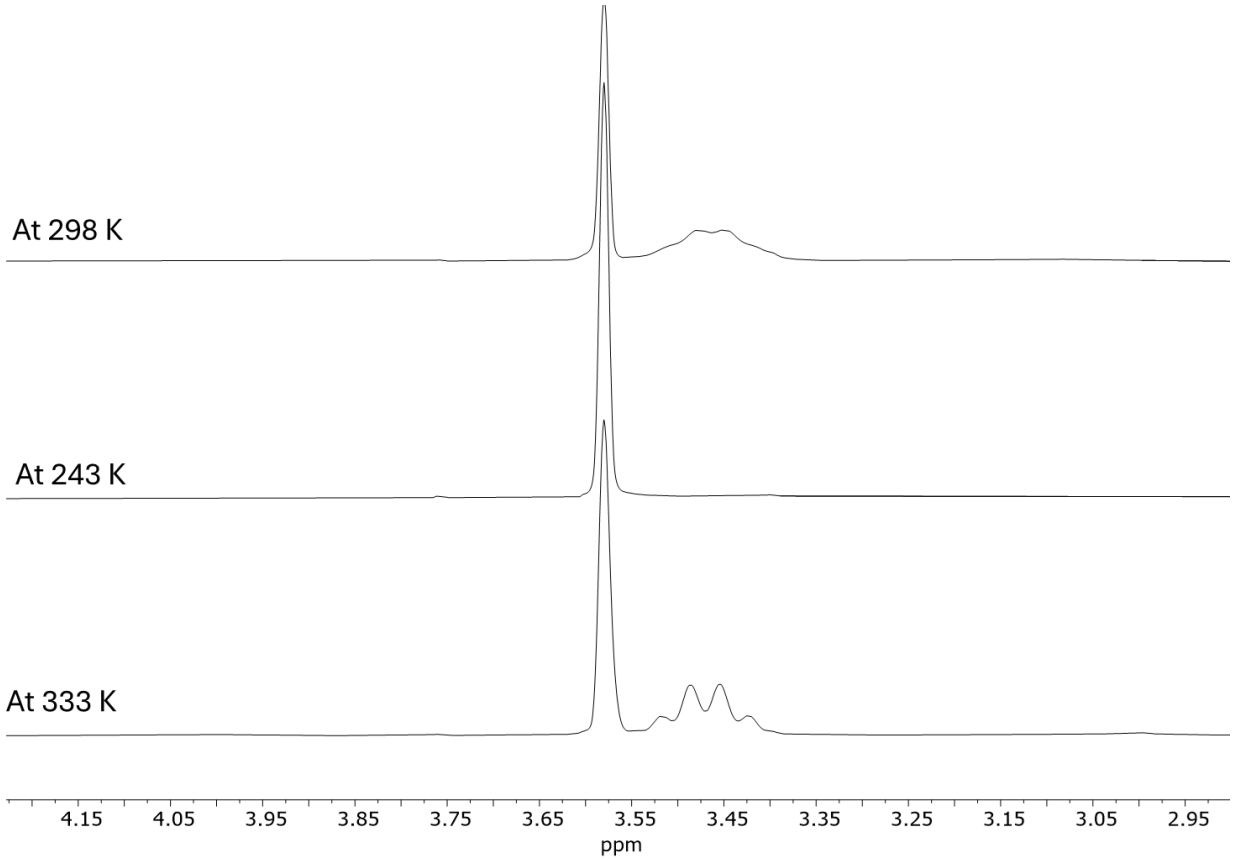


Figure S16. Excerpt from the stacked ^{1}H-NMR spectra of **6** measured in d_8-THF at 298 K (top), 243 K (middle) and 333 K (bottom), highlighting the temperature dependent behavior of the Cy-H *ipso*-signal.

4 Reactivity of silanone 6 towards CO_2

In a J-Young NMR tube, 20 mg (28.3 µmol, 1eq) **AYSi-2** were dissolved in d_8-THF (instead of toluene, see above) under an argon atmosphere, which was subsequently exchanged to 1.5 bar of N_2O, leading to immediate decolorization of the yellow solution. After shaking the tube for 4 h at RT, the atmosphere was again exchanged to 2 bar of CO_2. The next day the ^{1}H NMR spectrum displayed a slightly different shift pattern compared to silanone **6**, especially the Cy-H ipso signal was significantly altered by shifting from 3.46 ppm for **6** to 3.09 ppm in the obtained spectrum. This raised the question for the formation of a possible carbonate complex formation analogous to **8**. While the ^{13}C-NMR spectrum did not show the clear appearance of a C=O signal, the IR spectrum of the dried reaction mixture showed a band of low intensity at 1773 cm^{-1}, which could be interpreted as originating from a C=O stretching mode. In the IR spectrums of **AYSi-2** and **6** no band was observed at a comparable wavenumber. XRD analysis of crystals obtained from the reaction mixture only showed the structure of the silanone. However, the formation of the **AYSi-2** carbonate complex cannot be entirely ruled out but is likely to occur only as a minor product.

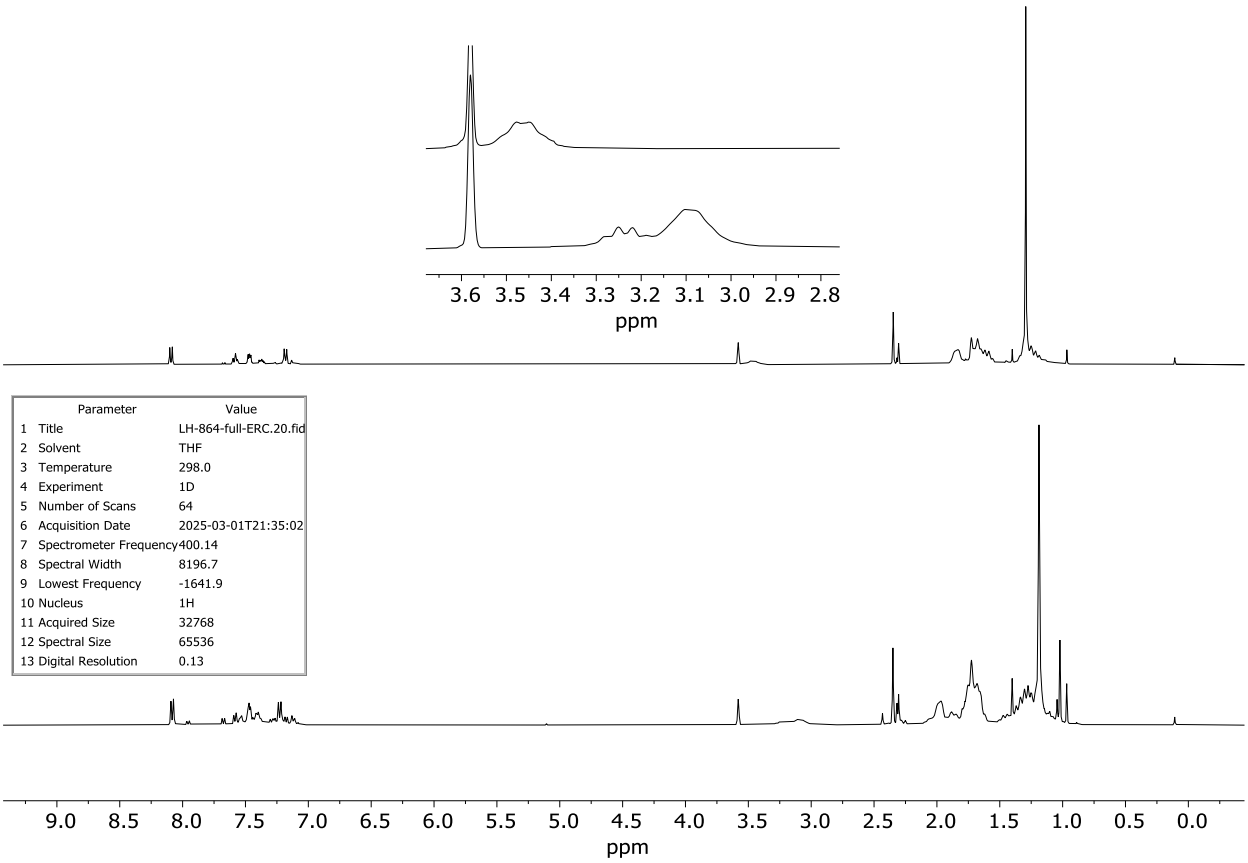


Figure S17. Stacked ^{1}H-NMR spectra of silanone **6** (top) and the CO_2 reaction mixture measured in d_8-THF. Highlighted in the expansion of the spectrum is the shifting of the Cy-H ipso signal.

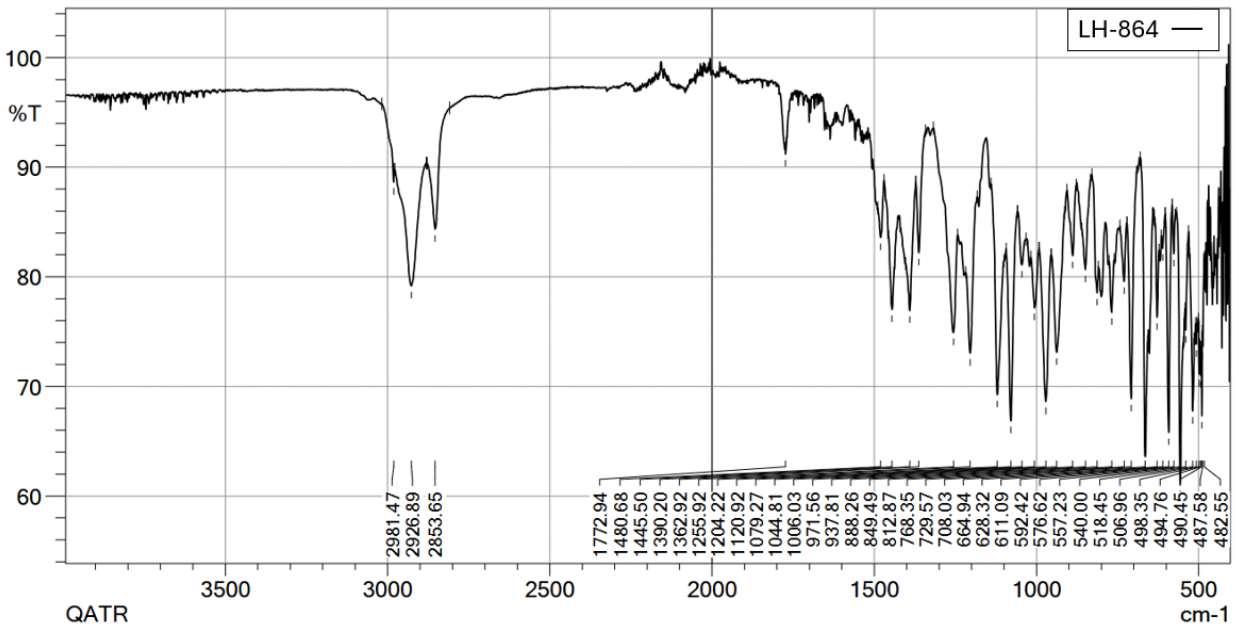


Figure S18. IR spectrum of the dried mixture from the reaction of **6** with CO_2.

5 NMR and IR Spectra of the Isolated Compounds

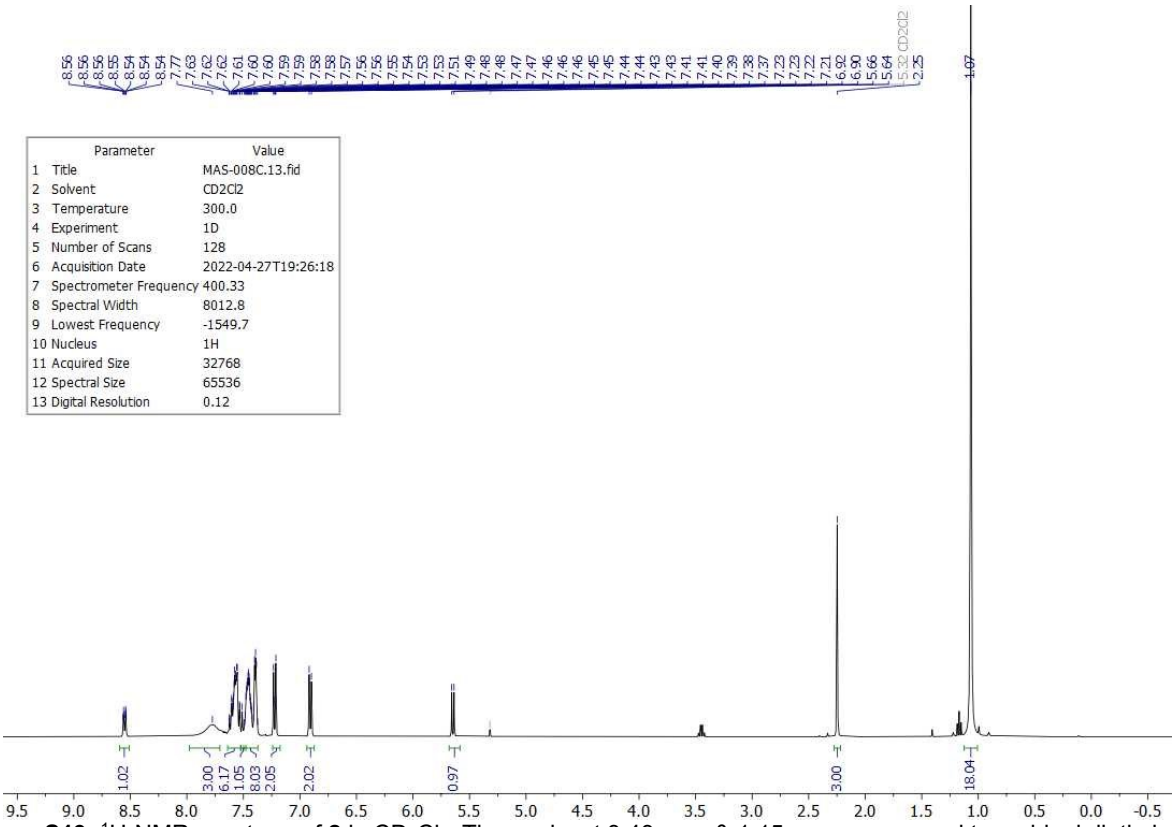


Figure S19. ^{1}H-NMR spectrum of **2** in CD_2Cl_2. The peaks at 3.43 ppm & 1.15 ppm correspond to residual diethyl ether.

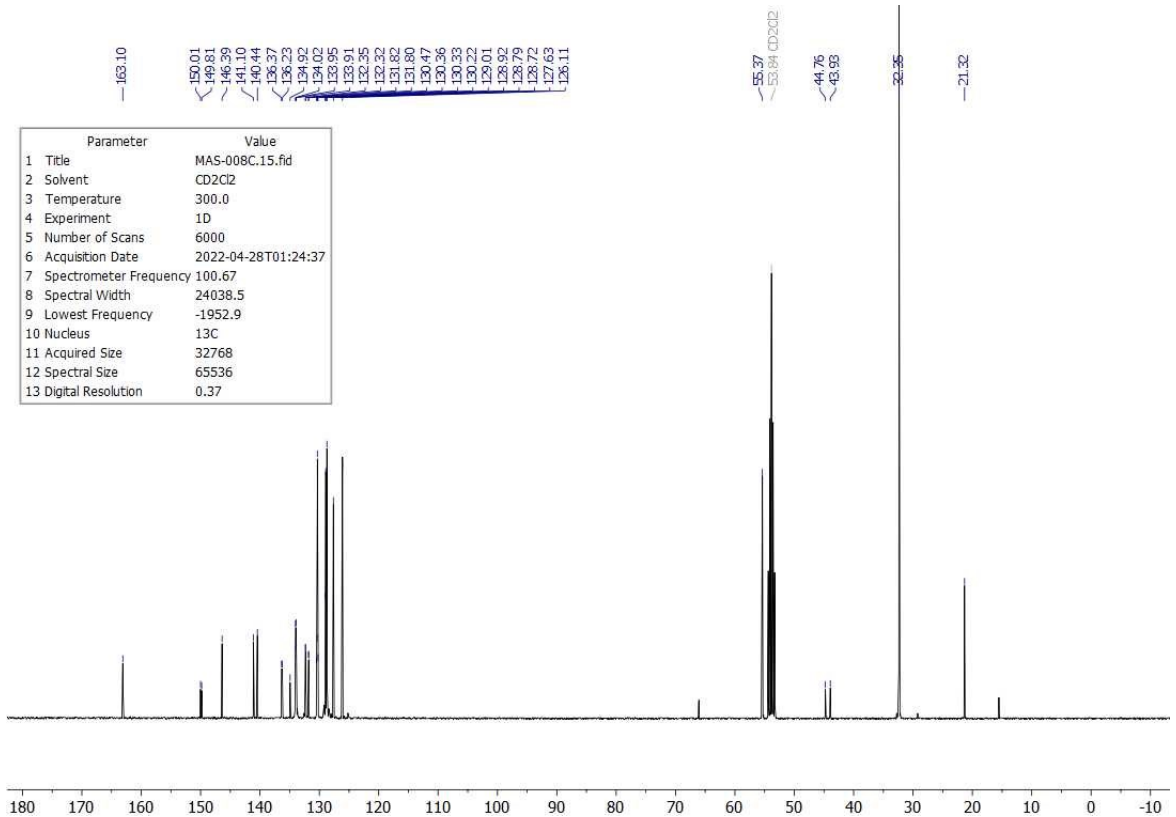


Figure S20. $^{13}C\{^{1}H\}$-NMR spectrum of **2** in CD_2Cl_2. The peaks at 66.1 ppm & 15.4 ppm correspond to residual diethyl ether.

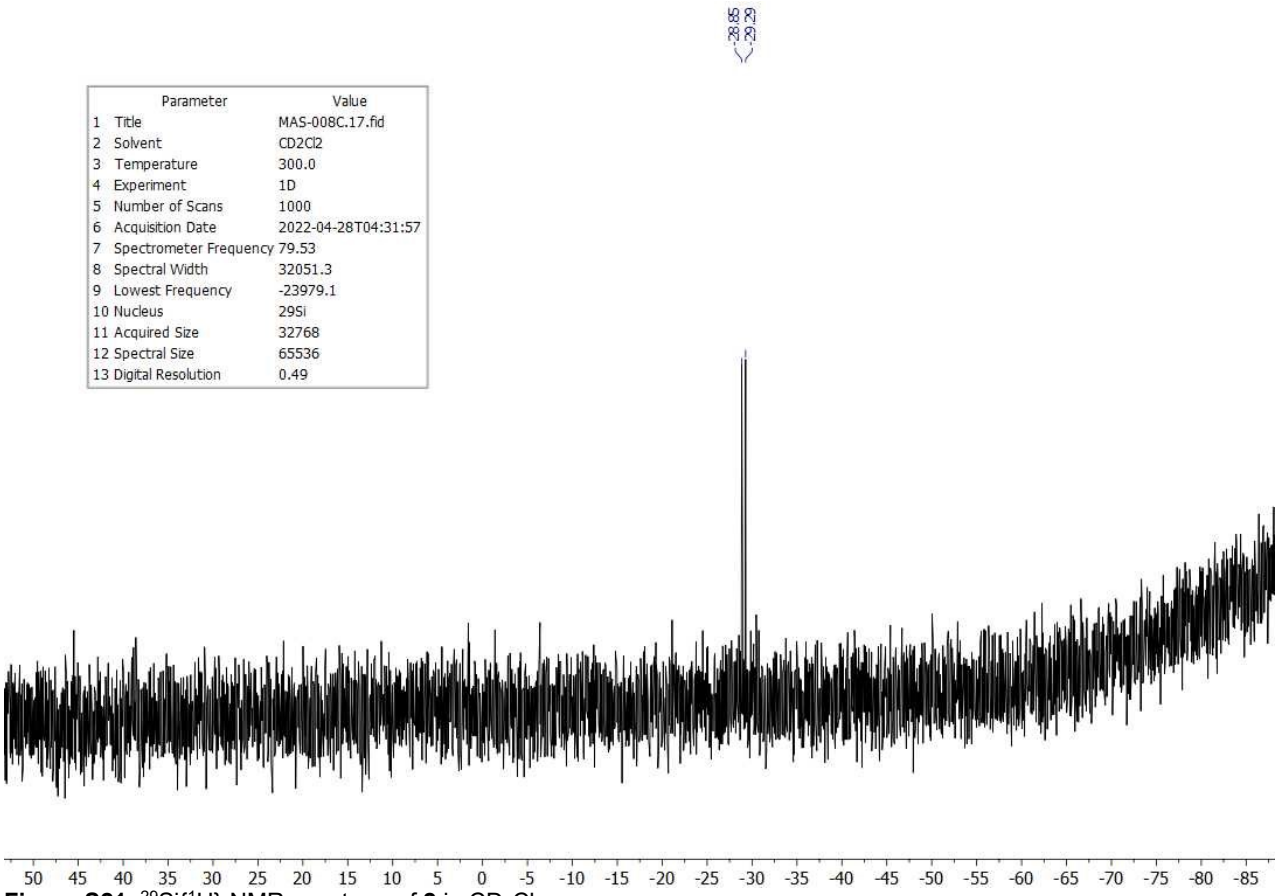


Figure S21. $^{29}Si\{^{1}H\}$-NMR spectrum of **2** in CD_2Cl_2.

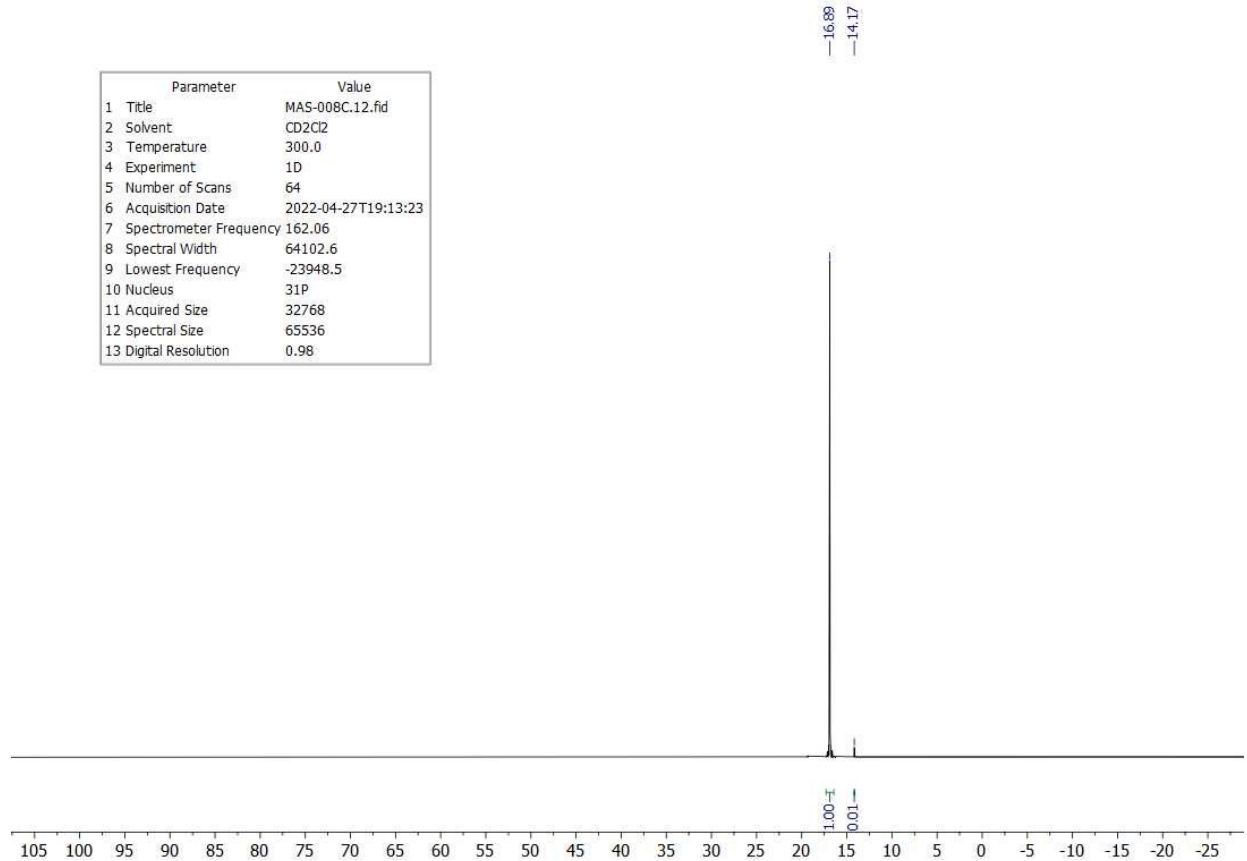


Figure S22. $^{31}P\{^{1}H\}$-NMR spectrum of **2** in C_6D_6. The peak at 14.2 ppm corresponds to the ylide.

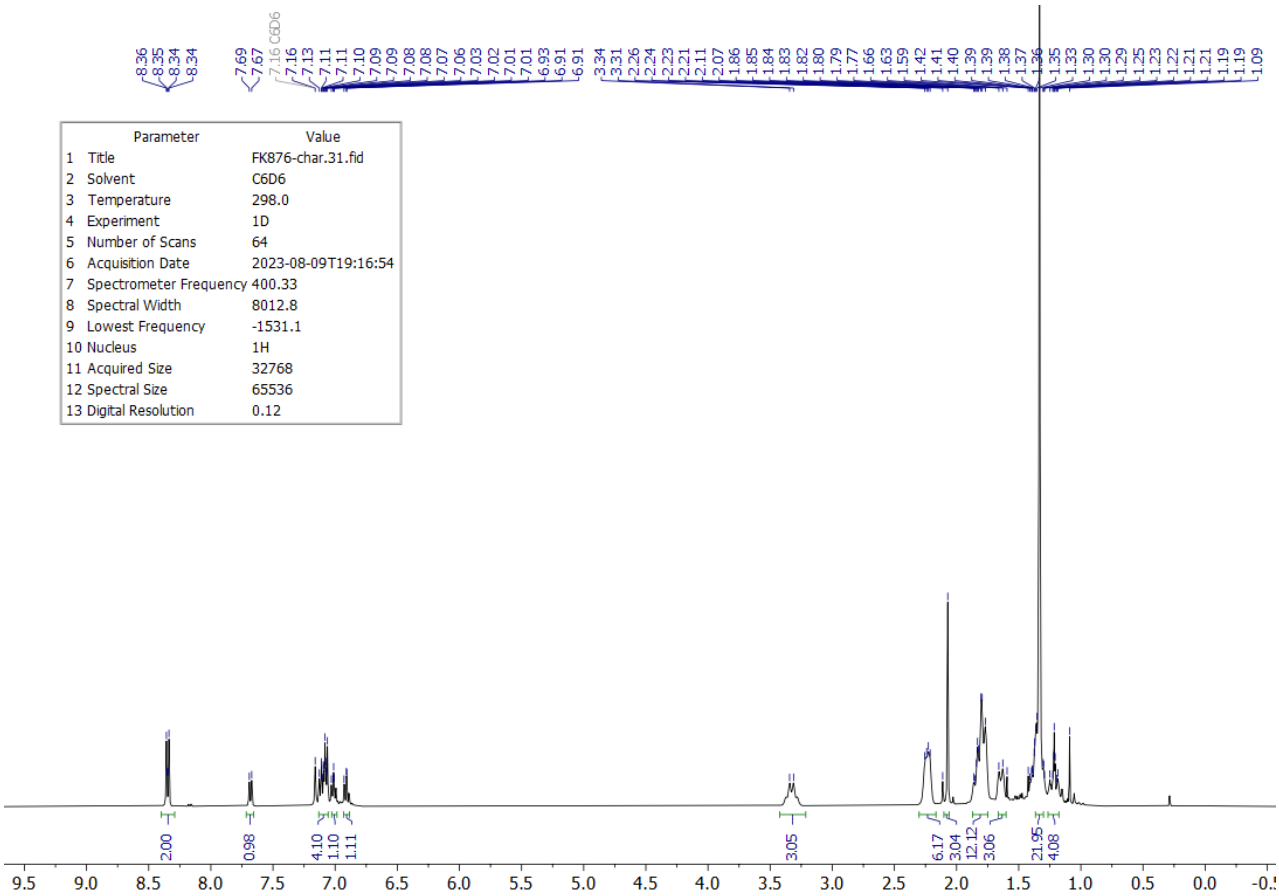


Figure S23. ^{1}H-NMR spectrum of **AYSi-2** in C_6D_6.

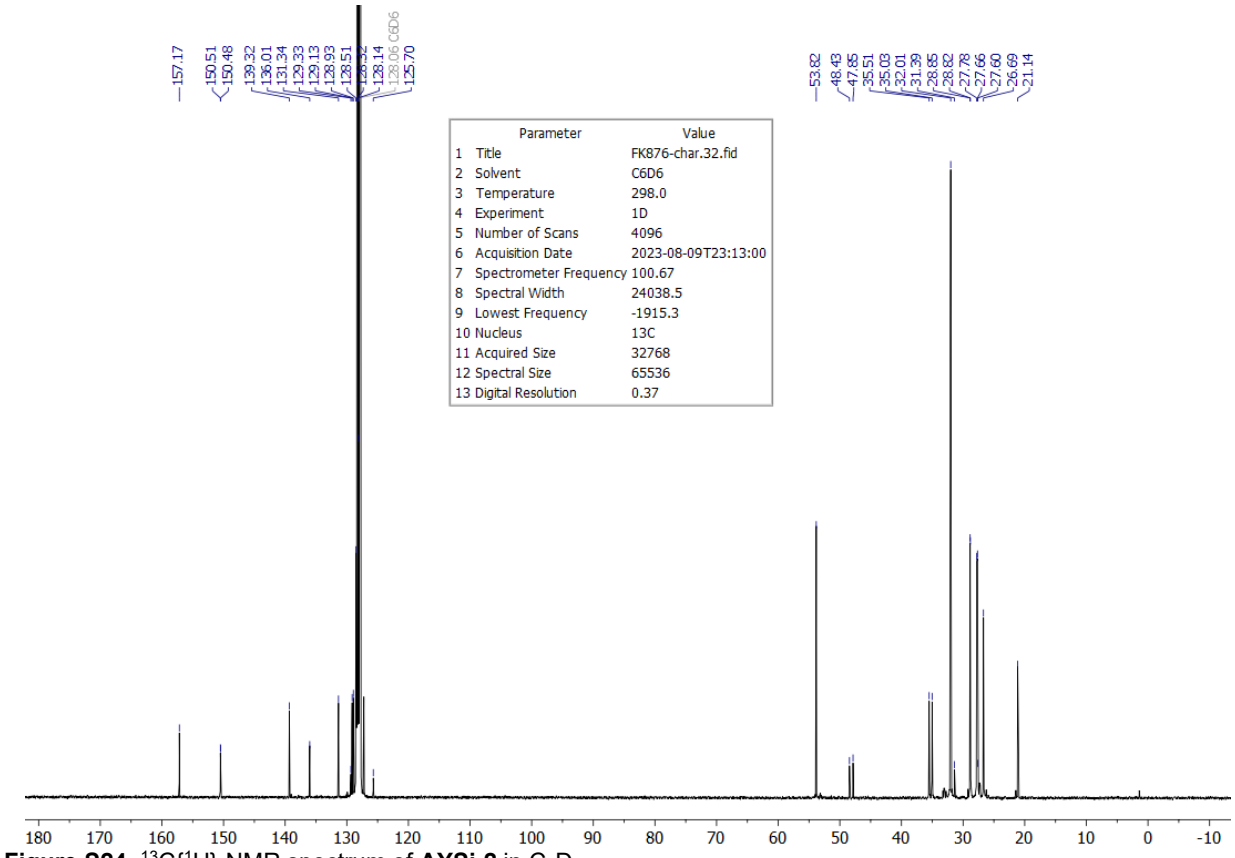


Figure S24. ^{13}C{^{1}H}-NMR spectrum of **AYSi-2** in C_6D_6.

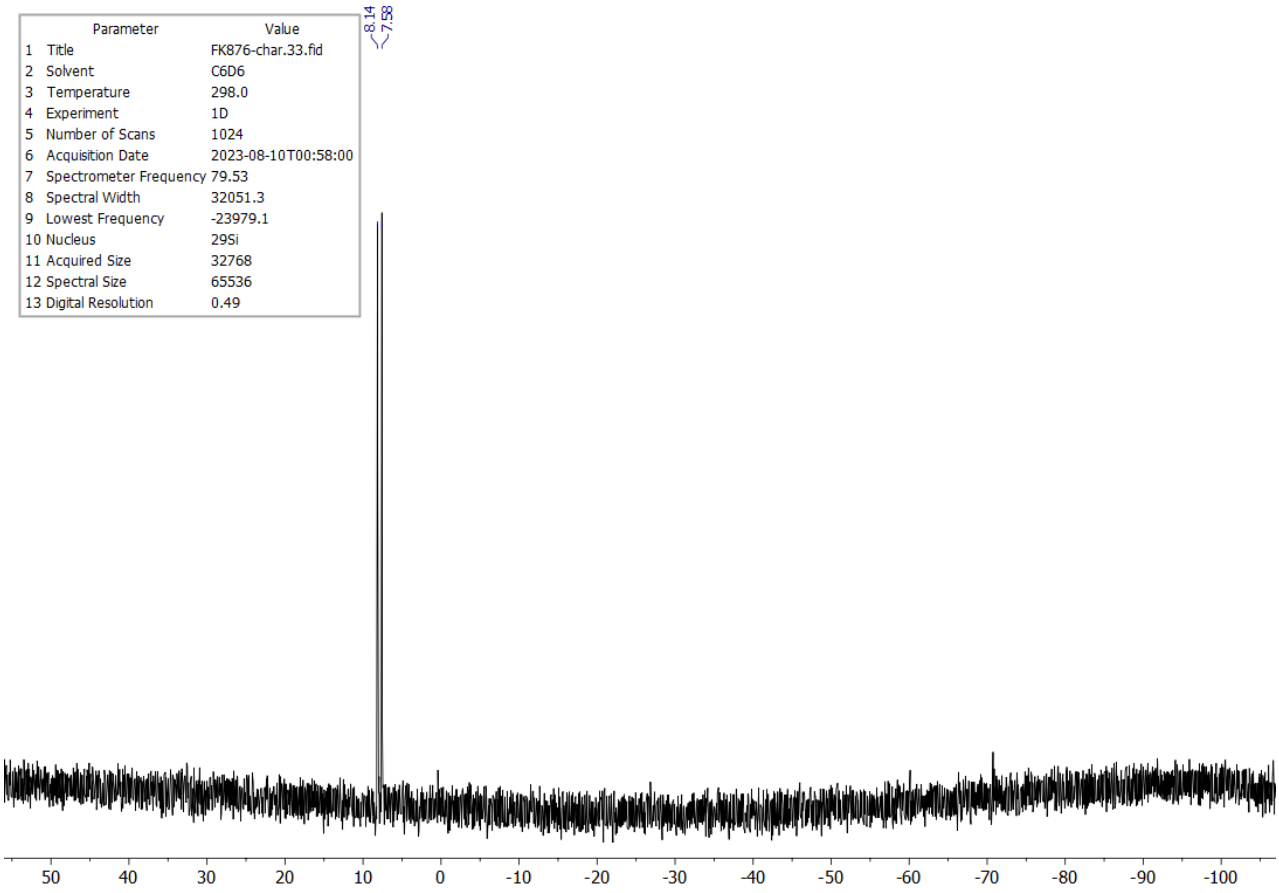


Figure S25. $^{29}Si\{^{1}H\}$-NMR spectrum of **AYSi-2** in C_6D_6.

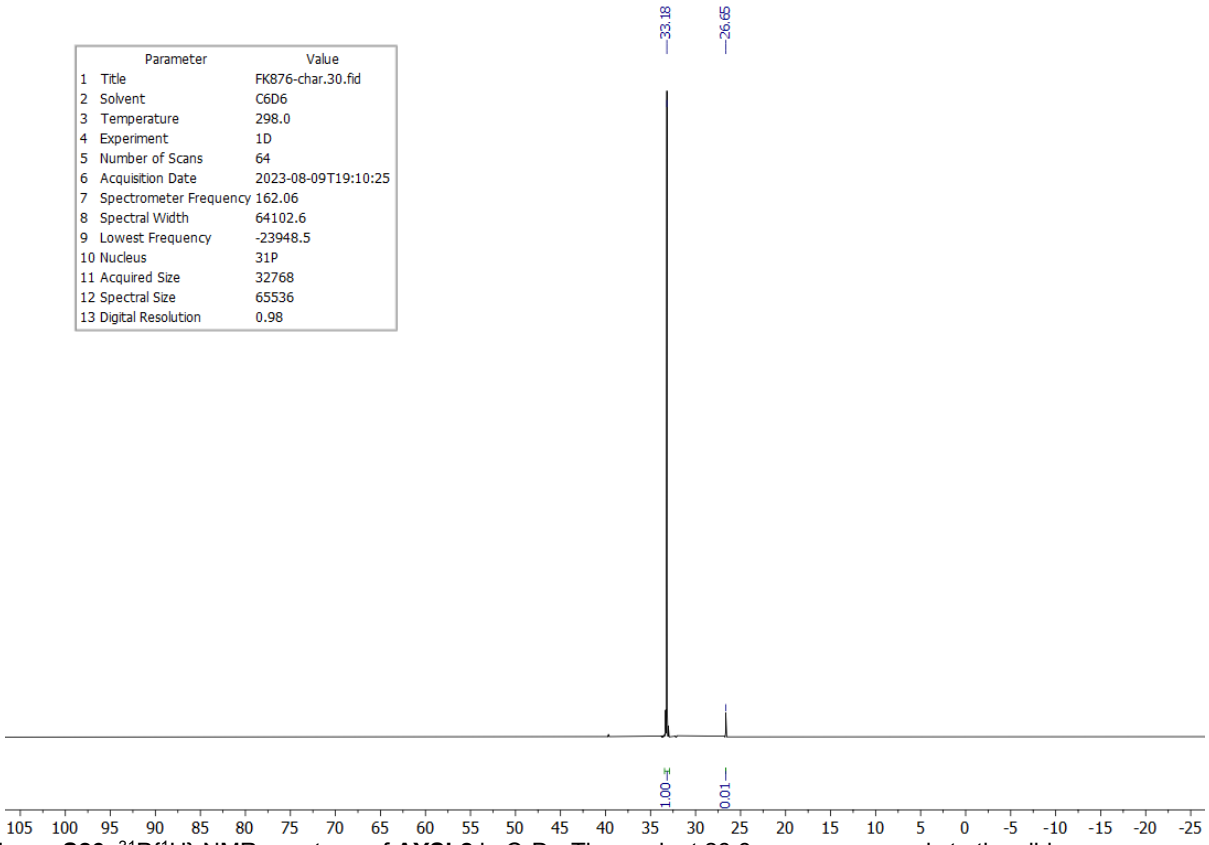


Figure S26. $^{31}P\{^{1}H\}$-NMR spectrum of **AYSi-2** in C_6D_6. The peak at 26.6 ppm corresponds to the ylide.

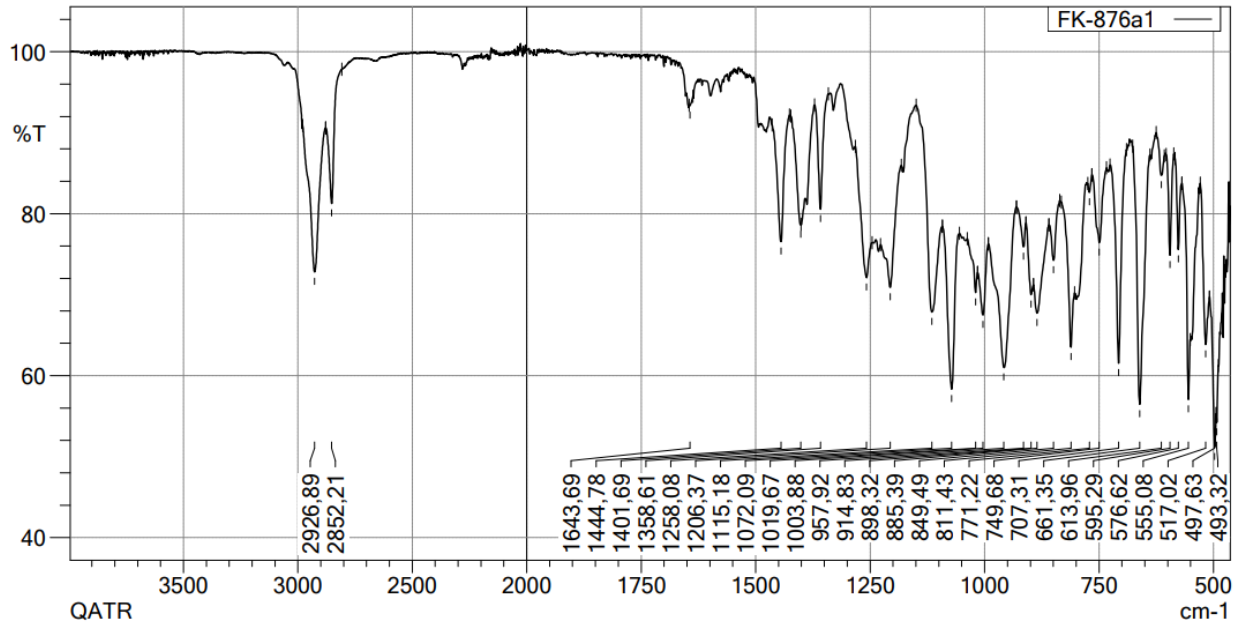


Figure S27. IR spectrum of solid **AYSi-2**.

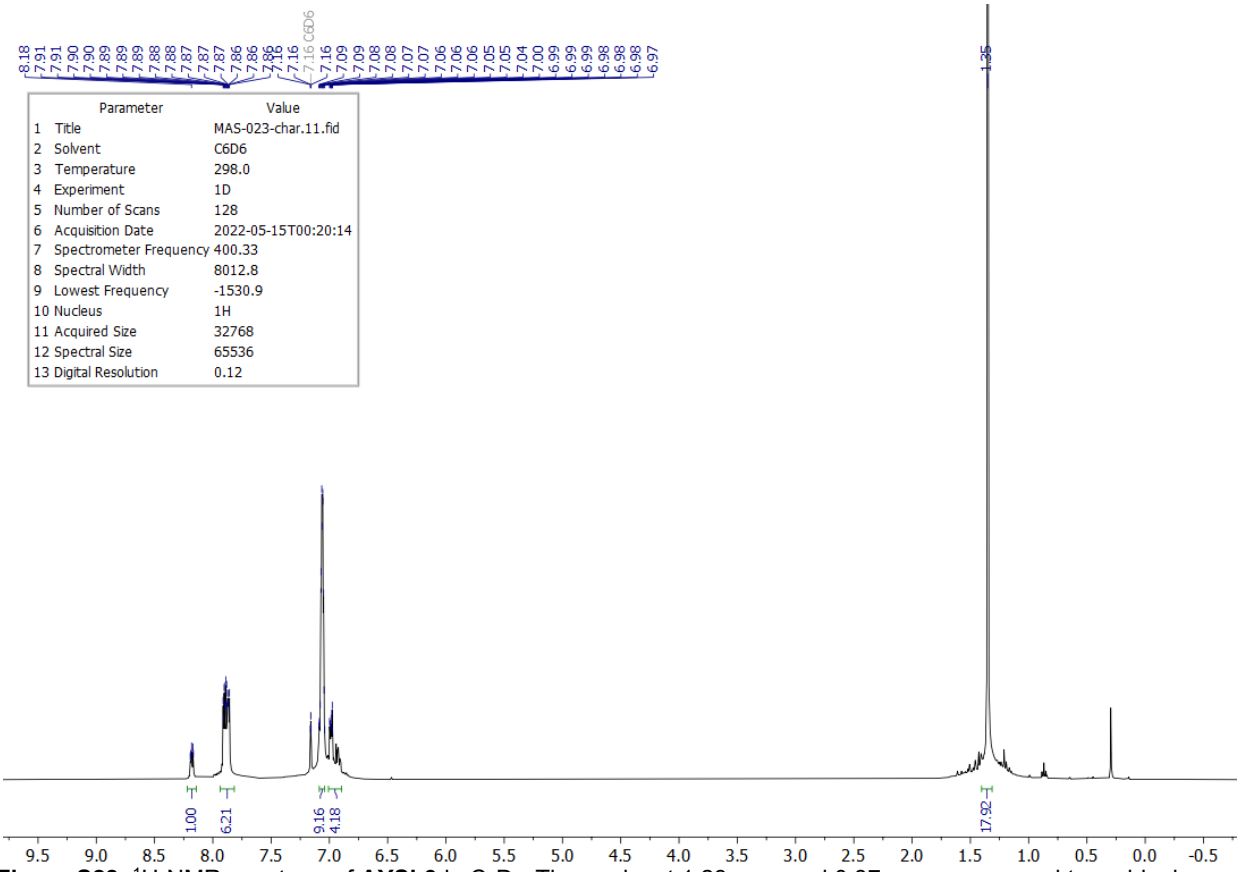


Figure S28. ^{1}H-NMR spectrum of **AYSi-3** in C_6D_6. The peaks at 1.23 ppm and 0.87 ppm correspond to residual pentane.

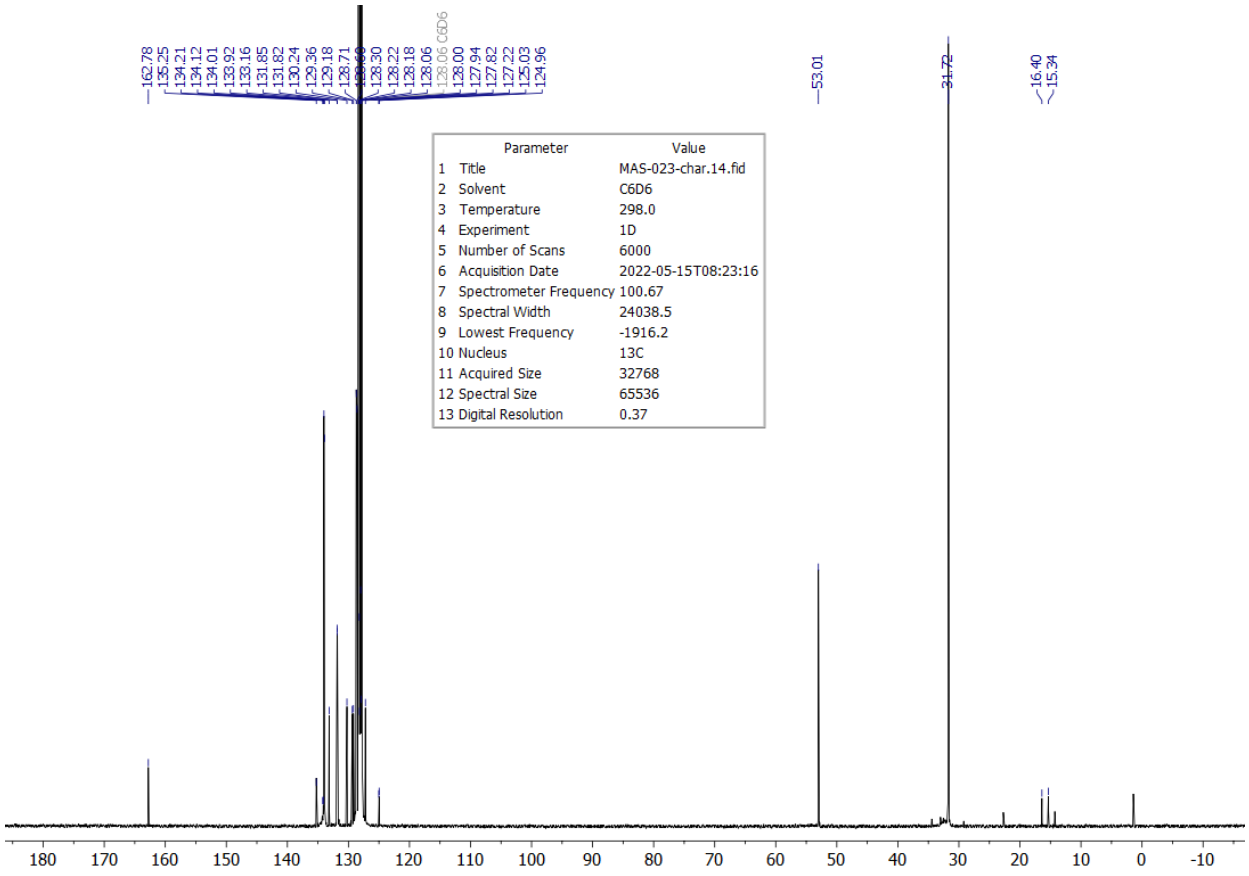


Figure S29. $^{13}C\{^{1}H\}$-NMR spectrum of **AYSi-3** in C_6D_6. The peaks at 34.5, 22.8 and 14.3 ppm correspond to residual pentane.

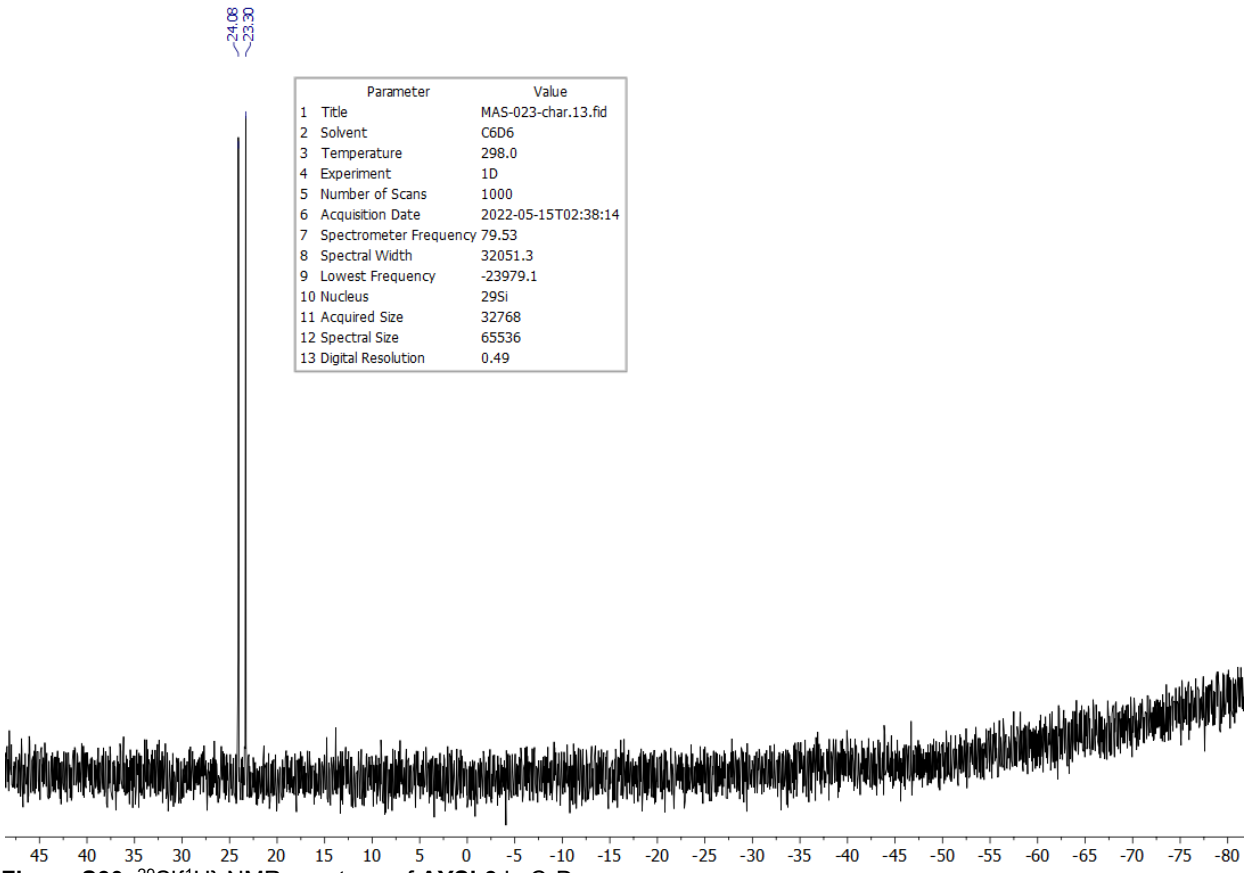


Figure S30. $^{29}Si\{^{1}H\}$-NMR spectrum of **AYSi-3** in C_6D_6.

	Parameter	Value
1	Title	MAS-023-char.10.fid
2	Solvent	C6D6
3	Temperature	298.0
4	Experiment	1D
5	Number of Scans	64
6	Acquisition Date	2022-05-15T00:06:50
7	Spectrometer Frequency	162.06
8	Spectral Width	64102.6
9	Lowest Frequency	-23948.5
10	Nucleus	31P
11	Acquired Size	32768
12	Spectral Size	65536
13	Digital Resolution	0.98

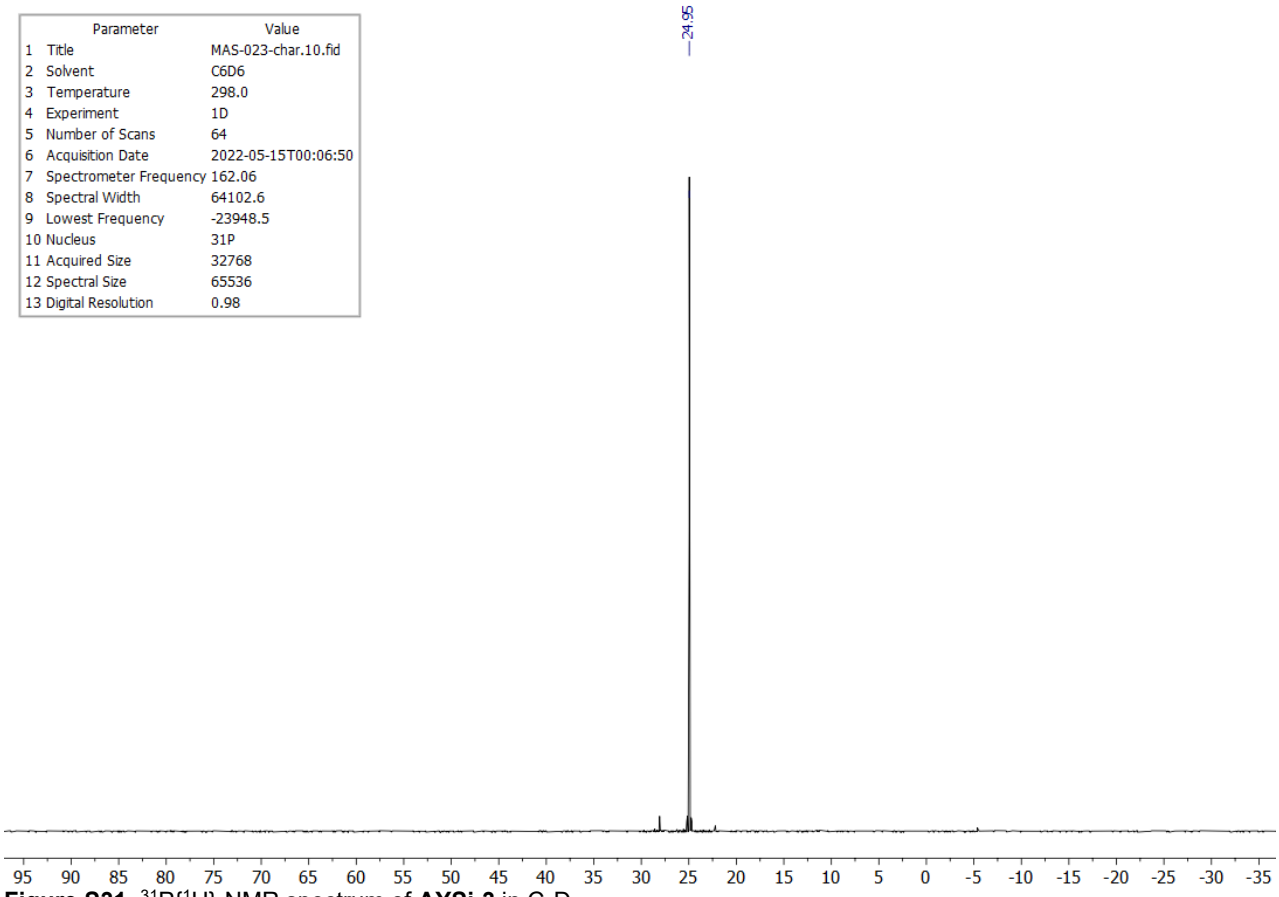


Figure S31. $^{31}P\{^{1}H\}$-NMR spectrum of **AYSi-3** in C_6D_6.

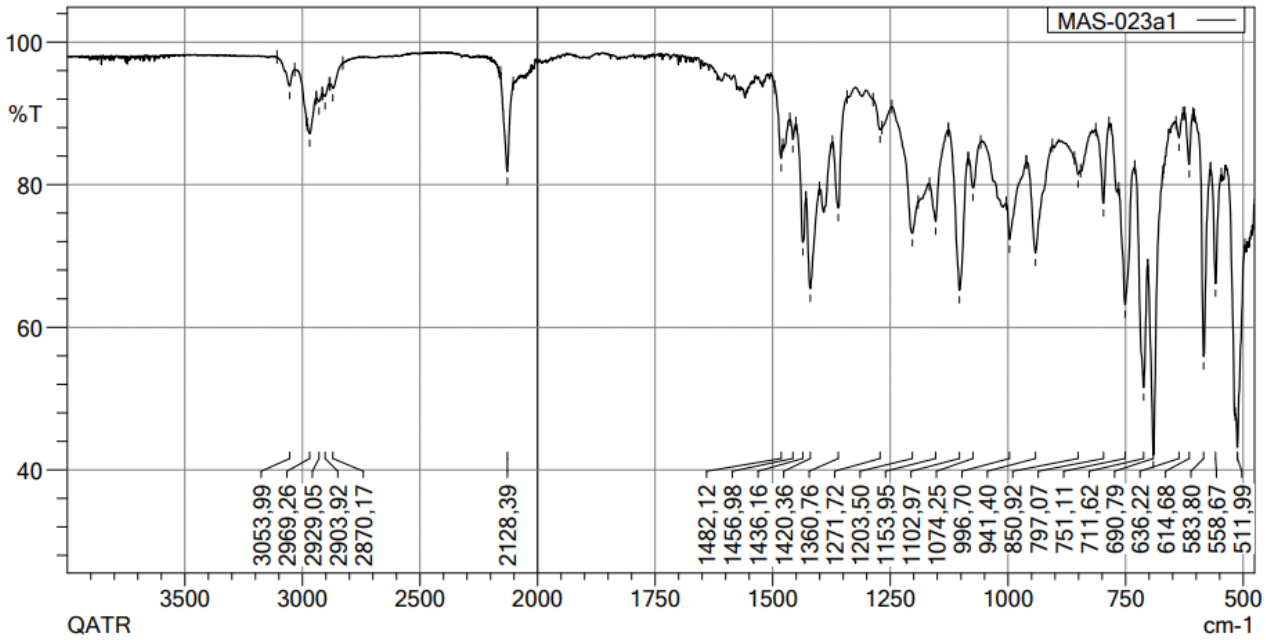


Figure S32. IR-spectrum of solid **AYSi-3**.

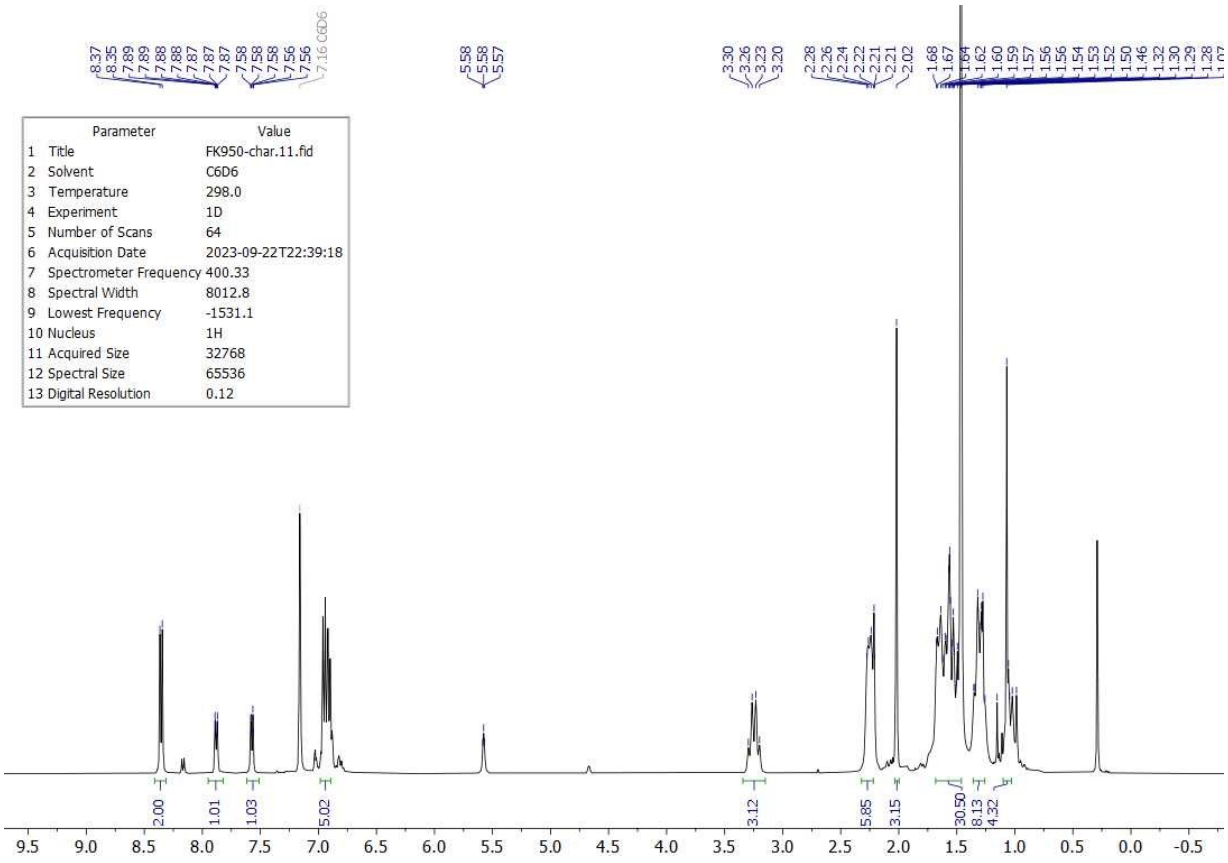


Figure S33. ^{1}H-NMR spectrum of **3** in C_6D_6. The peaks at 5.58 ppm and 2.21 ppm correspond to residual 1,5-cyclooctadiene. The peak 0.26 ppm corresponds to silicon grease.

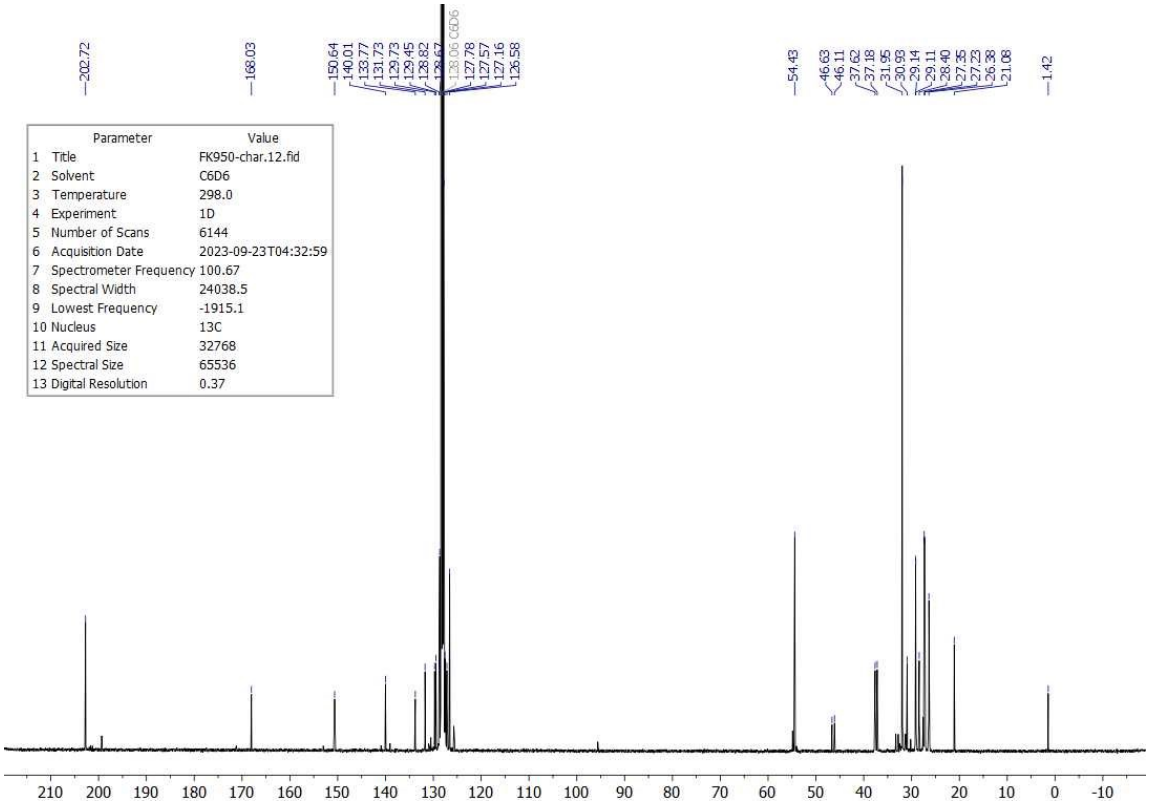


Figure S34. ^{13}C{^{1}H}-NMR spectrum of **3** in C_6D_6. The peaks at 128.8 ppm and 28.4 ppm correspond to 1,5-cyclooctadiene. The peak at 1.4 ppm corresponds to silicon grease.

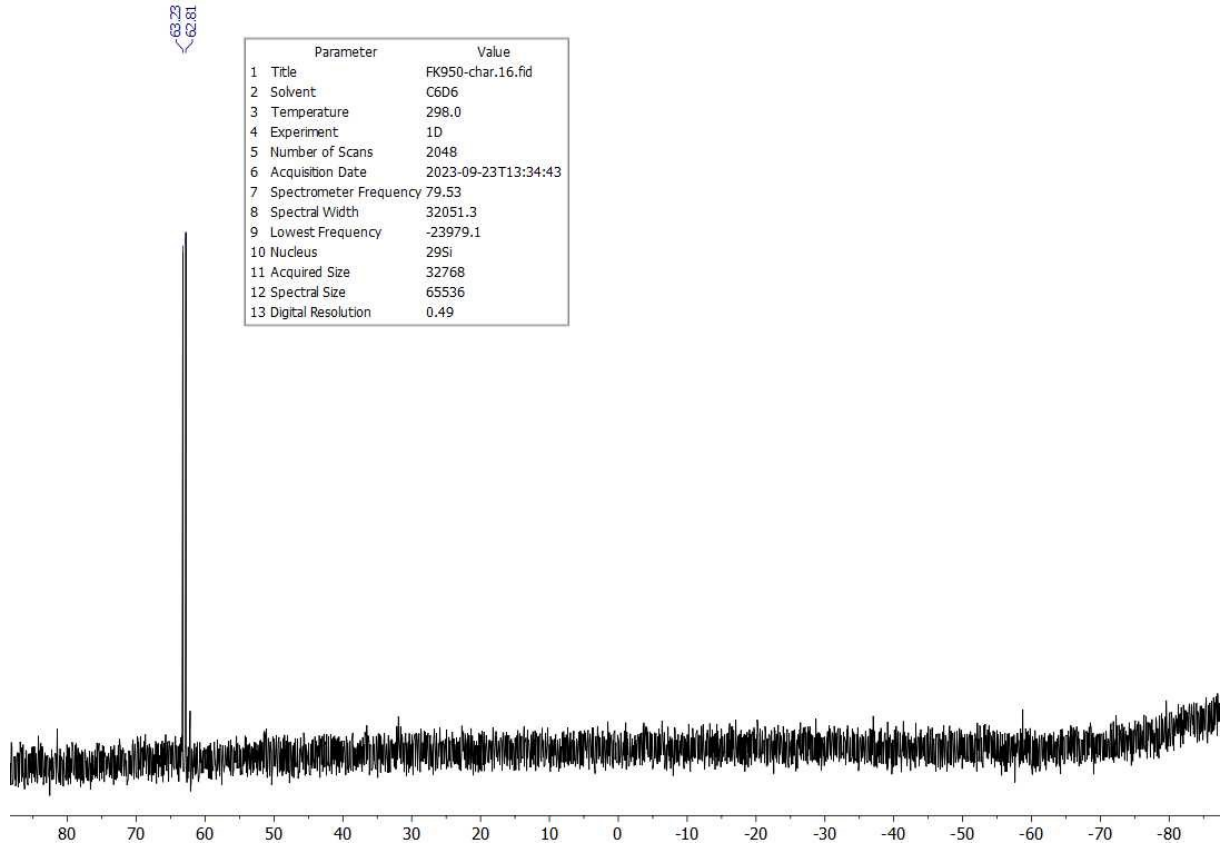


Figure S35. $^{29}Si\{^{1}H\}$-NMR spectrum of **3** in C_6D_6.

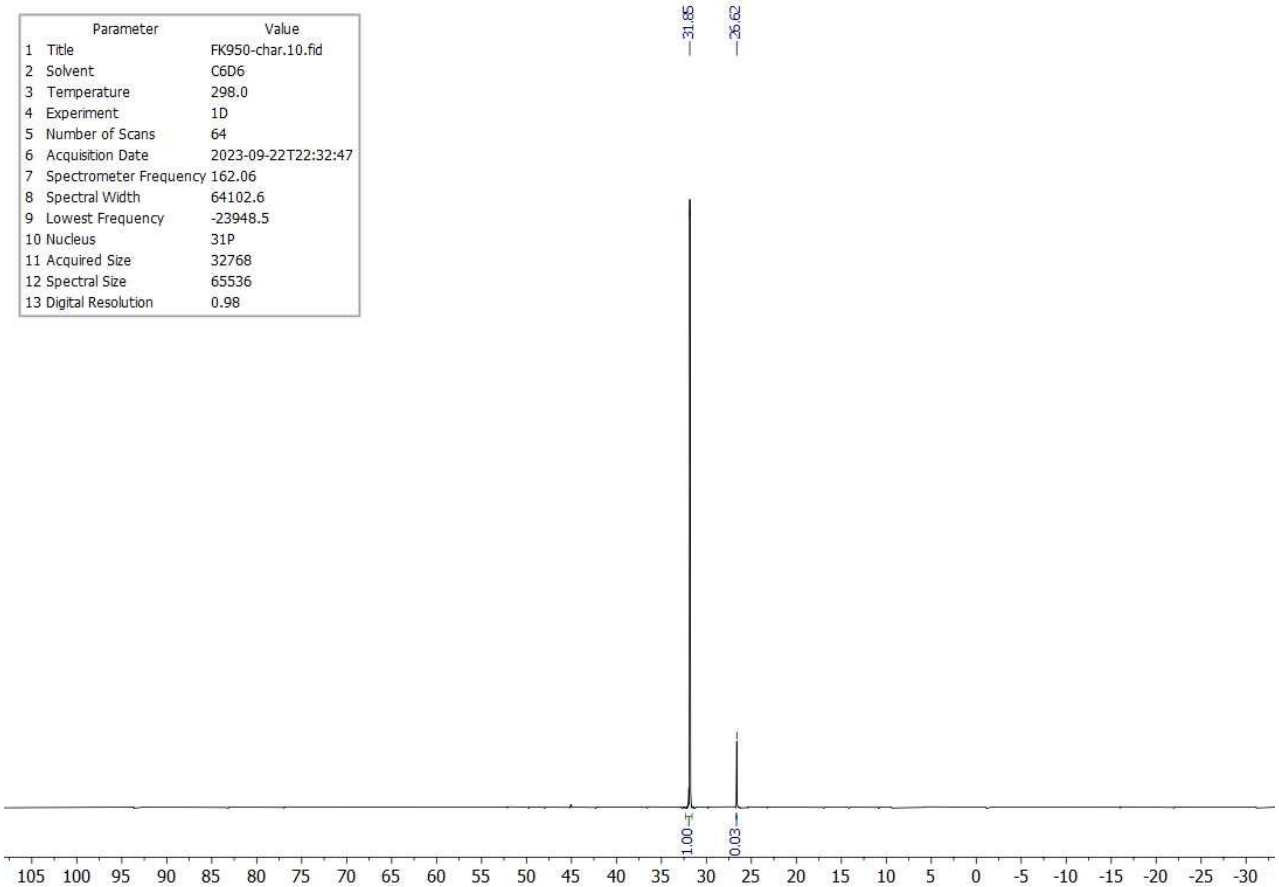


Figure S36. $^{31}P\{^{1}H\}$-NMR spectrum of **3** in C_6D_6. The peak at 26.6 ppm corresponds to the ylide.

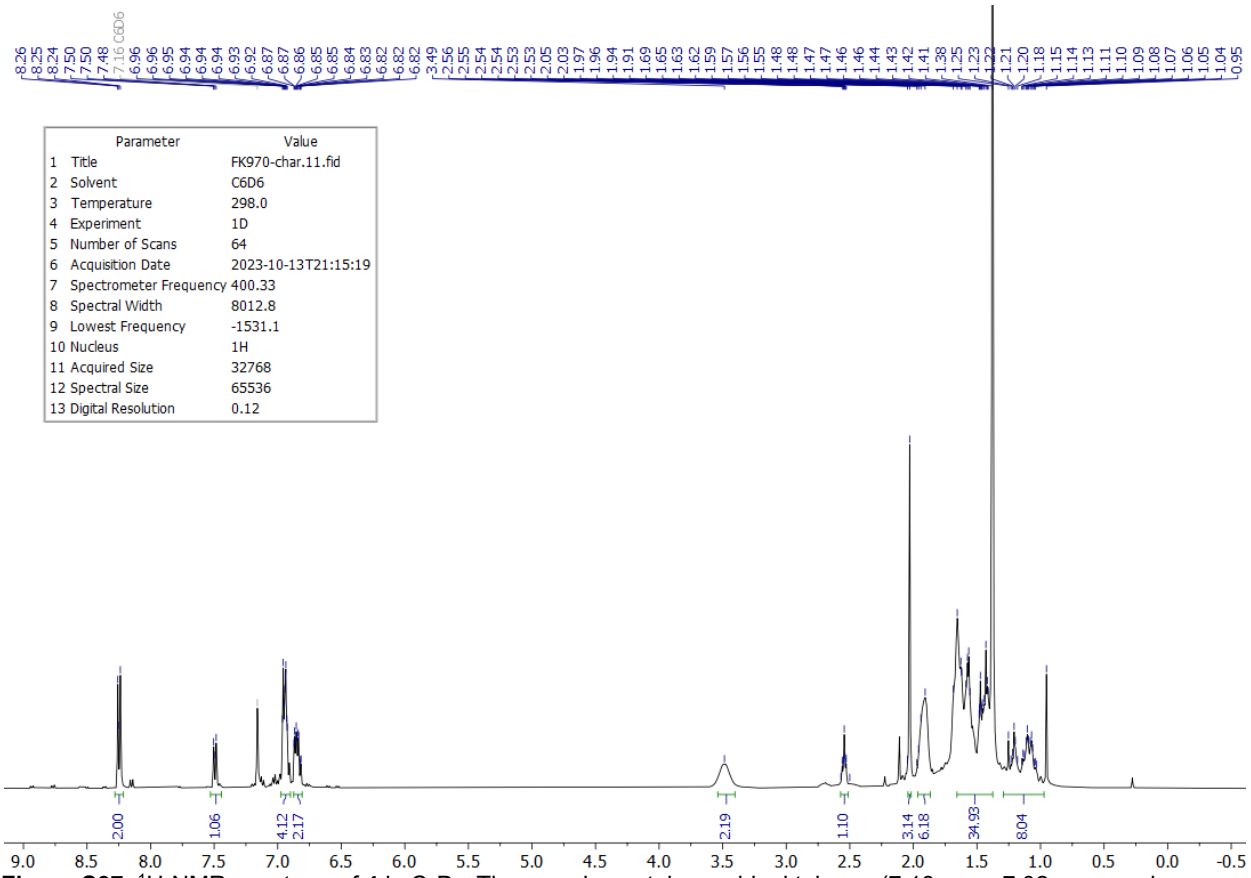


Figure S37. ^{1}H-NMR spectrum of **4** in C_6D_6. The sample contains residual toluene (7.13 ppm, 7.02 ppm, and 2.11 ppm).

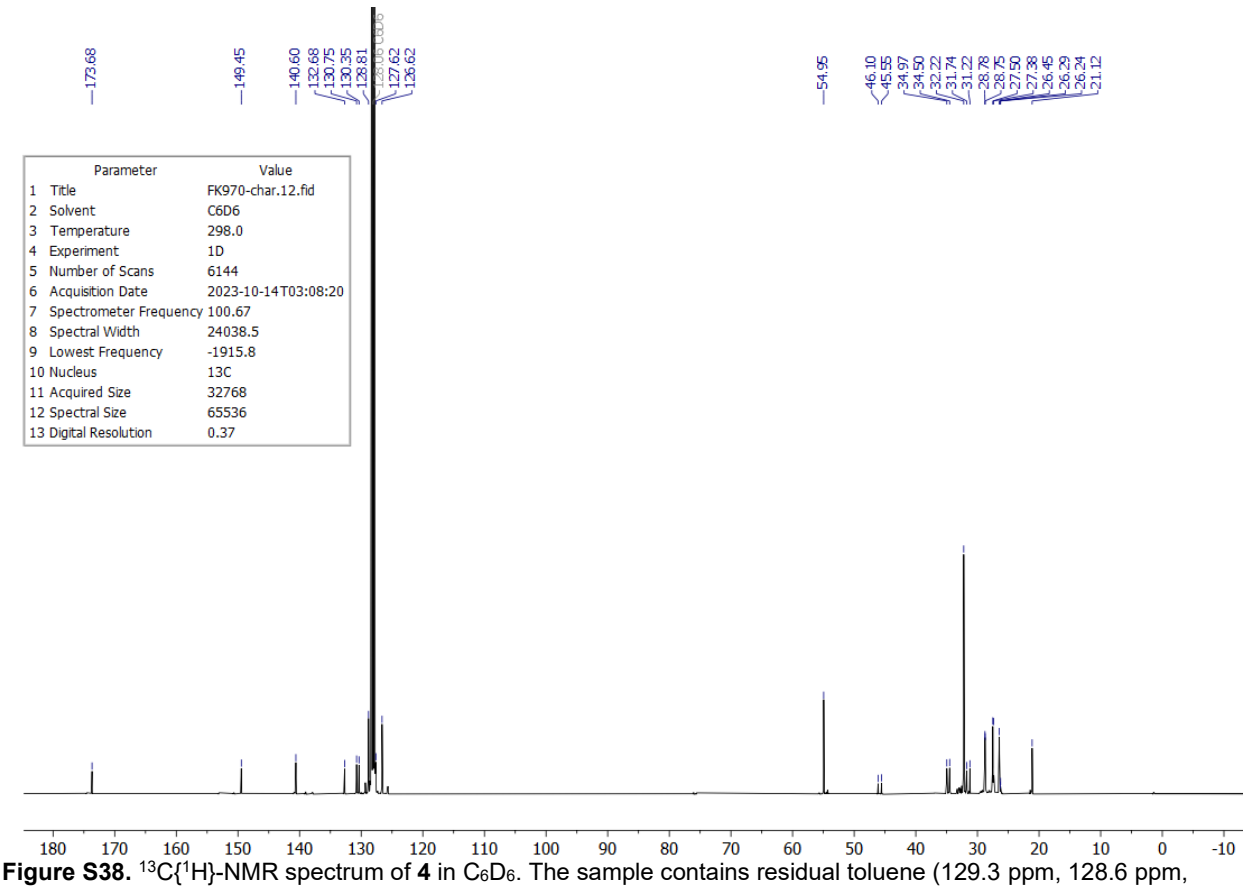


Figure S38. ^{13}C{^{1}H}-NMR spectrum of **4** in C_6D_6. The sample contains residual toluene (129.3 ppm, 128.6 ppm, 125.7 ppm, and 21.1 ppm).

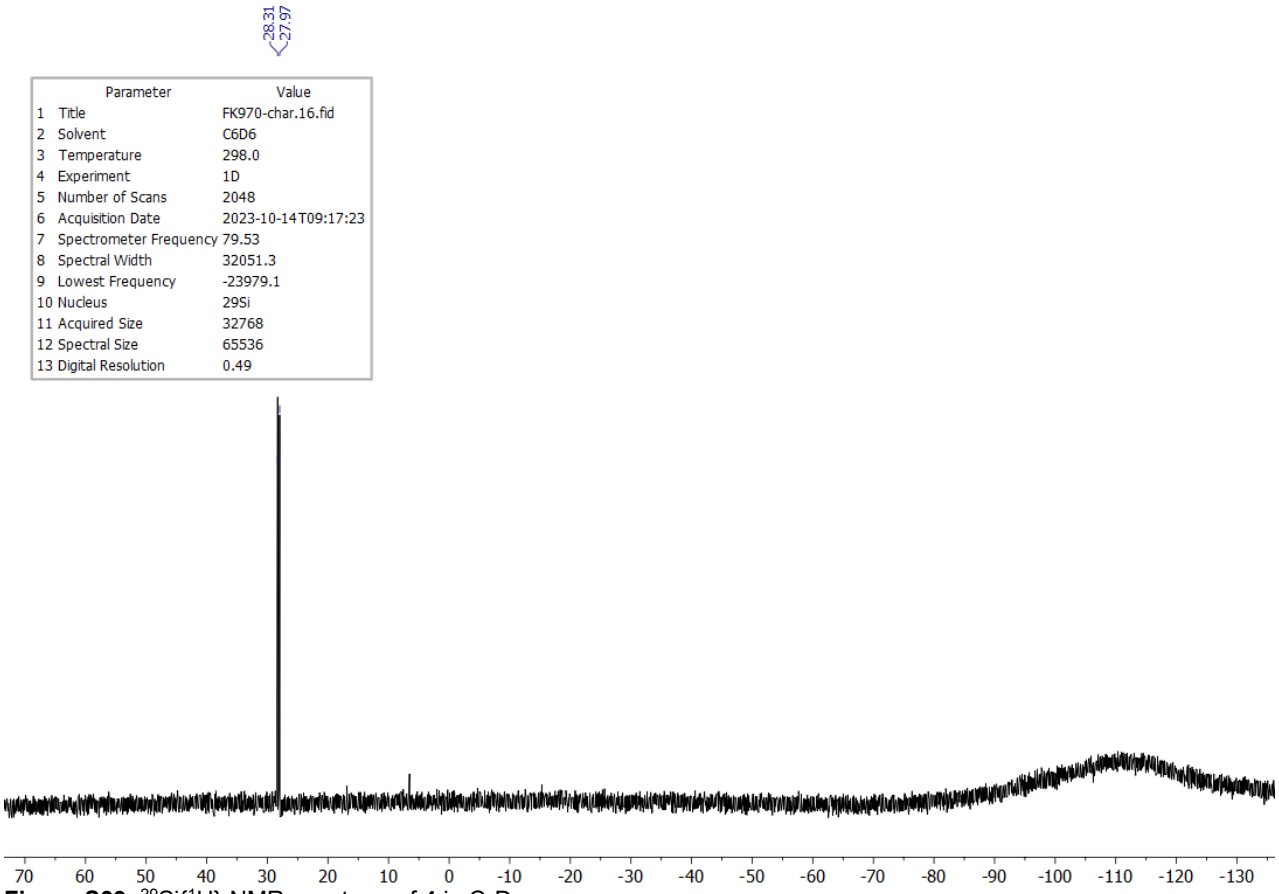


Figure S39. $^{29}Si\{^{1}H\}$-NMR spectrum of **4** in C_6D_6.

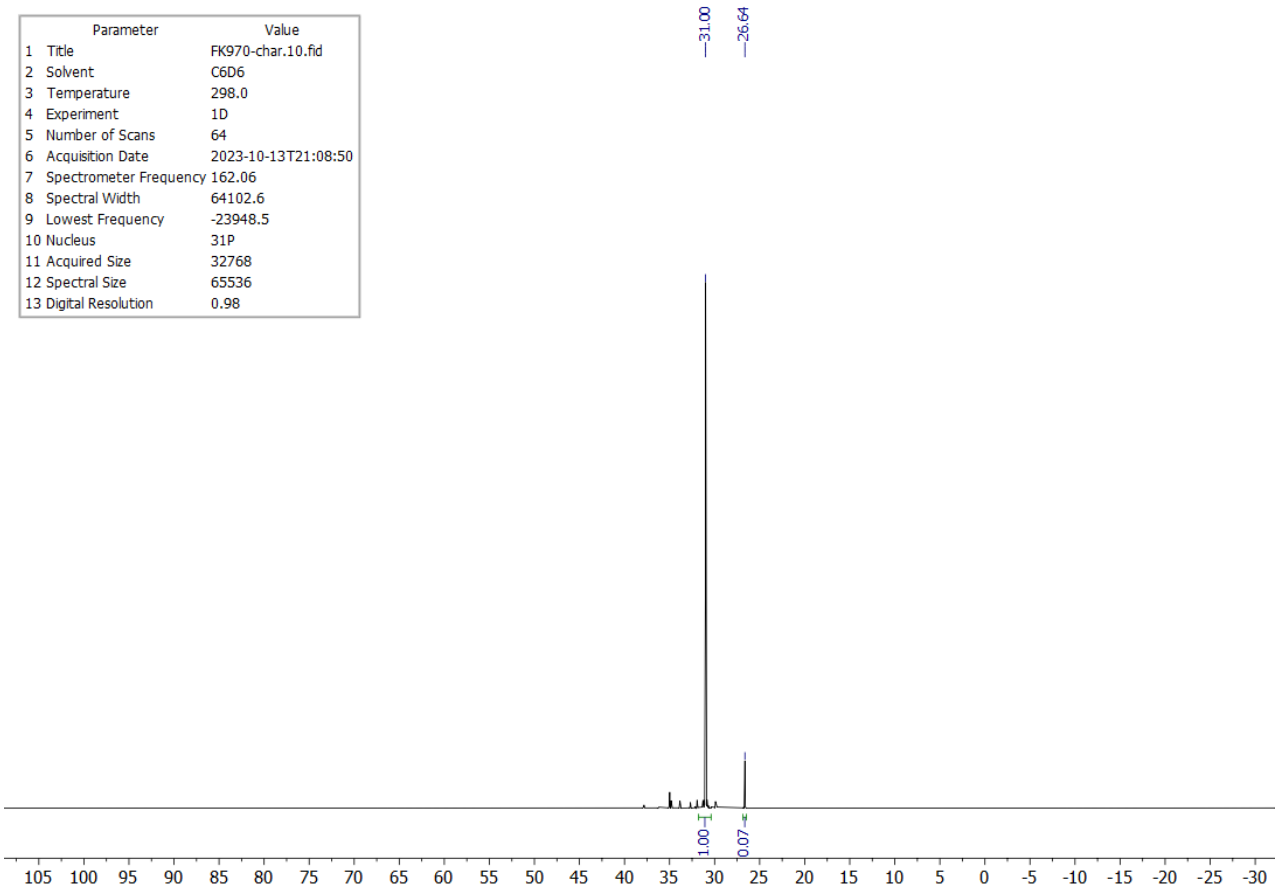
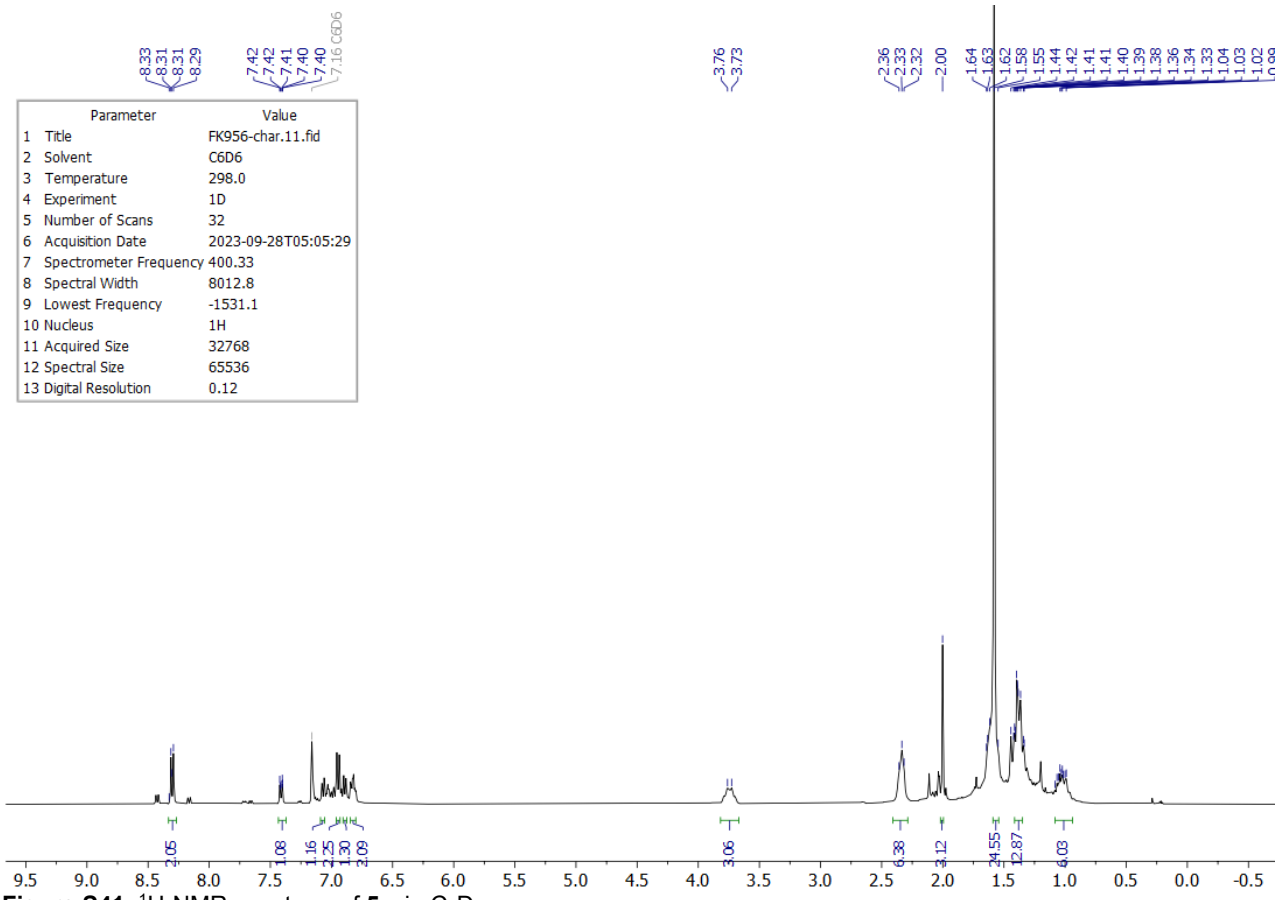
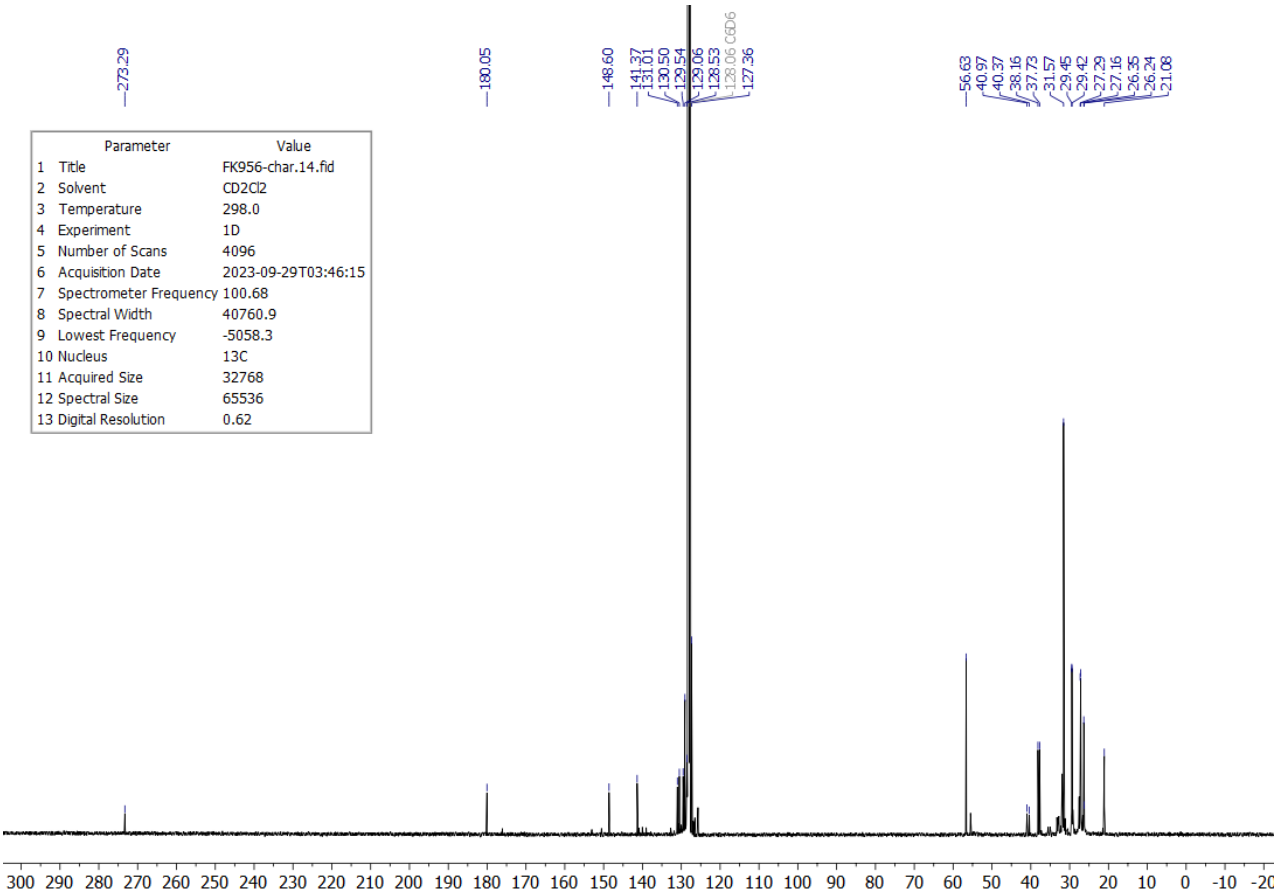


Figure S40. $^{31}P\{^{1}H\}$-NMR spectrum of **4** in C_6D_6. The peak at 26.6 ppm corresponds to the ylide.



	Parameter	Value
1	Title	FK956-char.11.fid
2	Solvent	C6D6
3	Temperature	298.0
4	Experiment	1D
5	Number of Scans	32
6	Acquisition Date	2023-09-28T05:05:29
7	Spectrometer Frequency	400.33
8	Spectral Width	8012.8
9	Lowest Frequency	-1531.1
10	Nucleus	1H
11	Acquired Size	32768
12	Spectral Size	65536
13	Digital Resolution	0.12

Figure S41. ^{1}H-NMR spectrum of **5$_{Ts}$** in C_6D_6.



	Parameter	Value
1	Title	FK956-char.14.fid
2	Solvent	CD2Cl2
3	Temperature	298.0
4	Experiment	1D
5	Number of Scans	4096
6	Acquisition Date	2023-09-29T03:46:15
7	Spectrometer Frequency	100.68
8	Spectral Width	40760.9
9	Lowest Frequency	-5058.3
10	Nucleus	13C
11	Acquired Size	32768
12	Spectral Size	65536
13	Digital Resolution	0.62

Figure S42. ^{13}C{^{1}H}-NMR spectrum of **5$_{Ts}$** in C_6D_6.

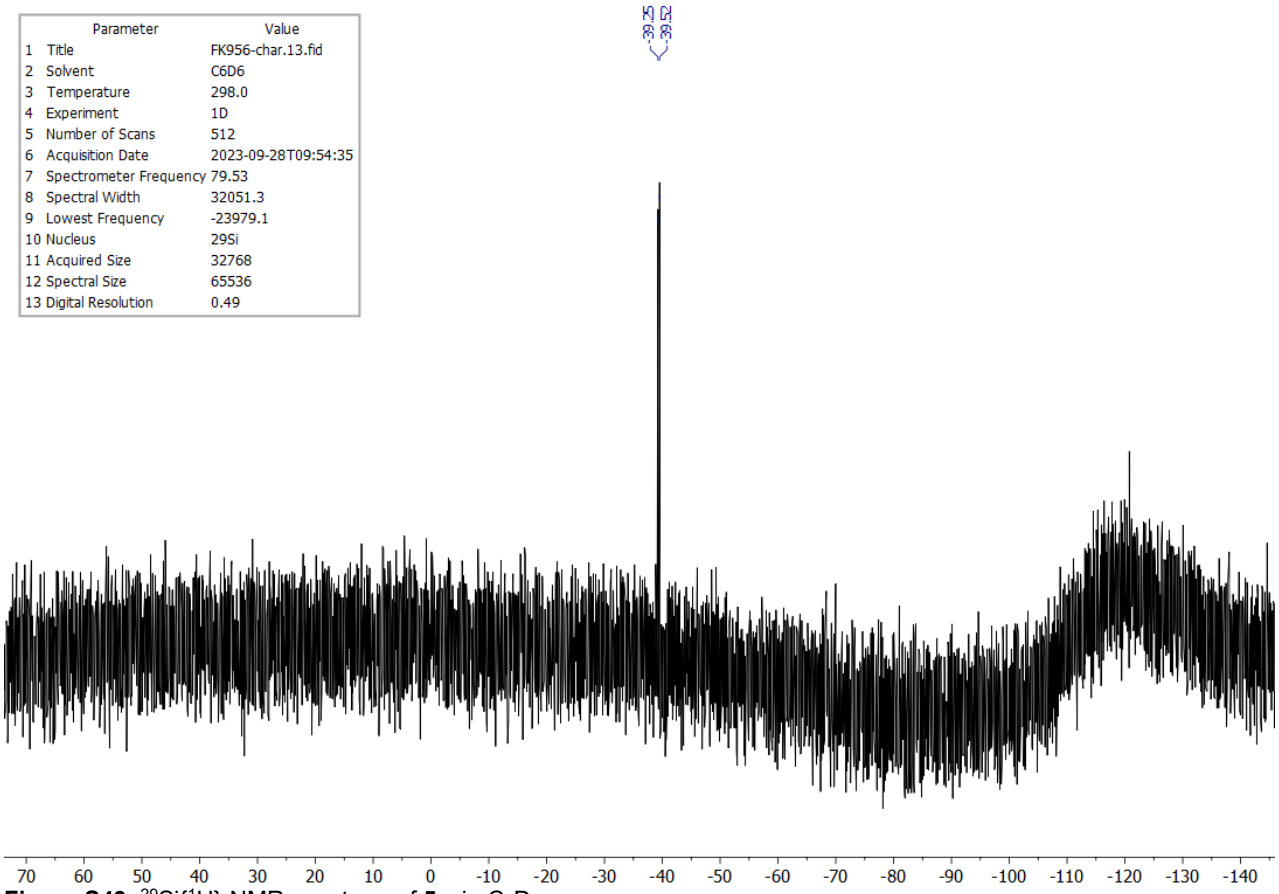


Figure S43. $^{29}Si\{^{1}H\}$-NMR spectrum of **5$_{Ts}$** in C_6D_5.

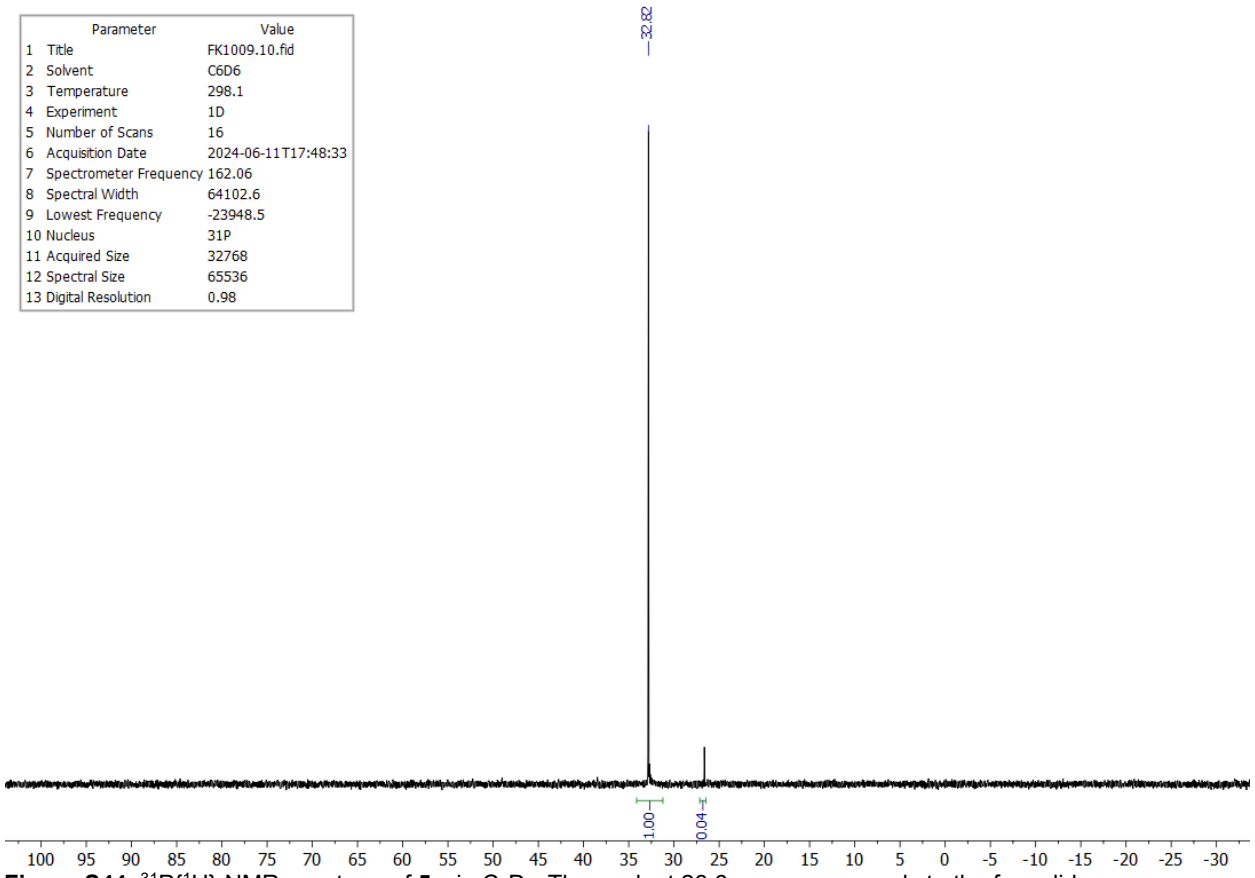


Figure S44. $^{31}P\{^{1}H\}$-NMR spectrum of **5$_{Ts}$** in C_6D_6. The peak at 26.6 ppm corresponds to the free ylide.

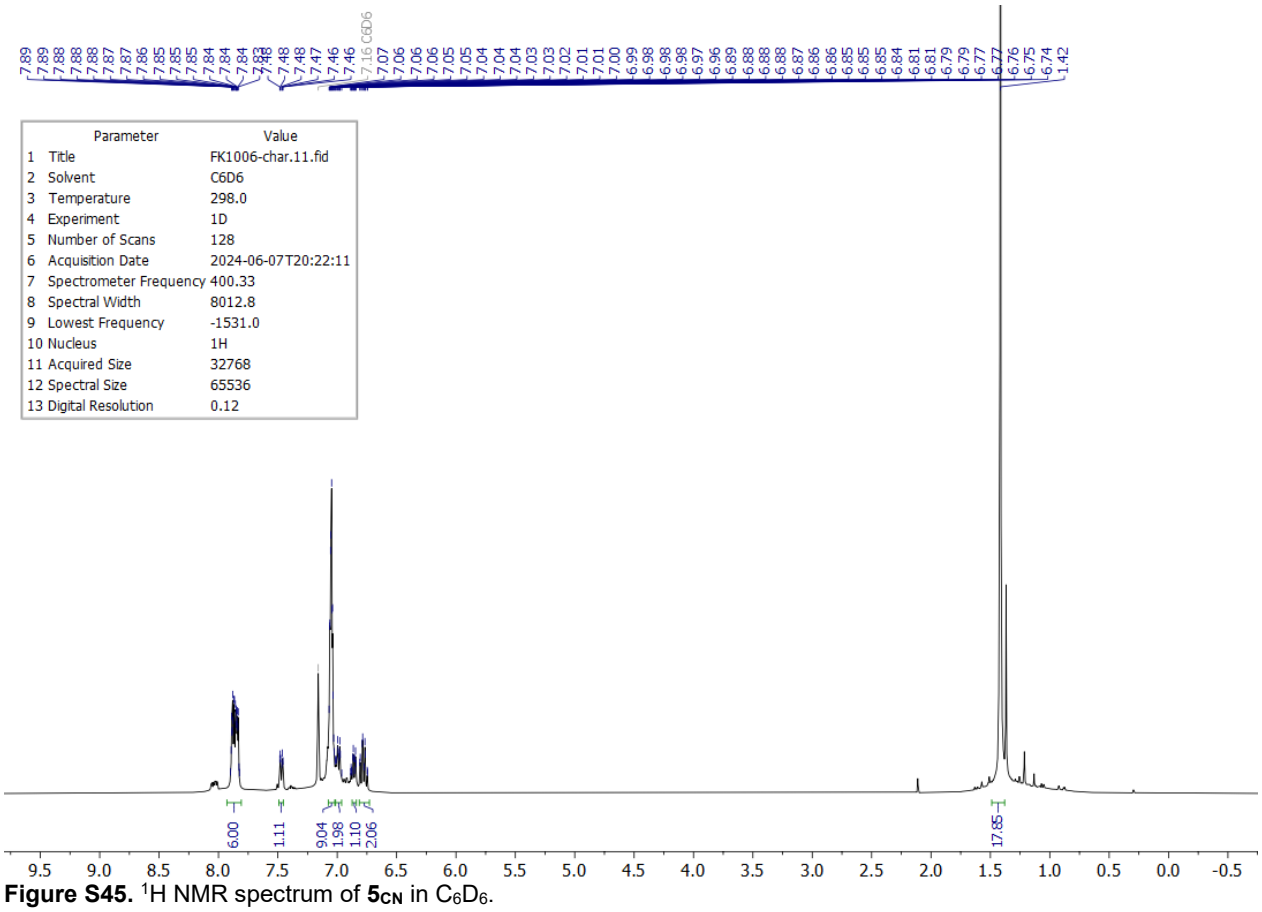


Figure S45. ^{1}H NMR spectrum of **5$_{CN}$** in C_6D_6.

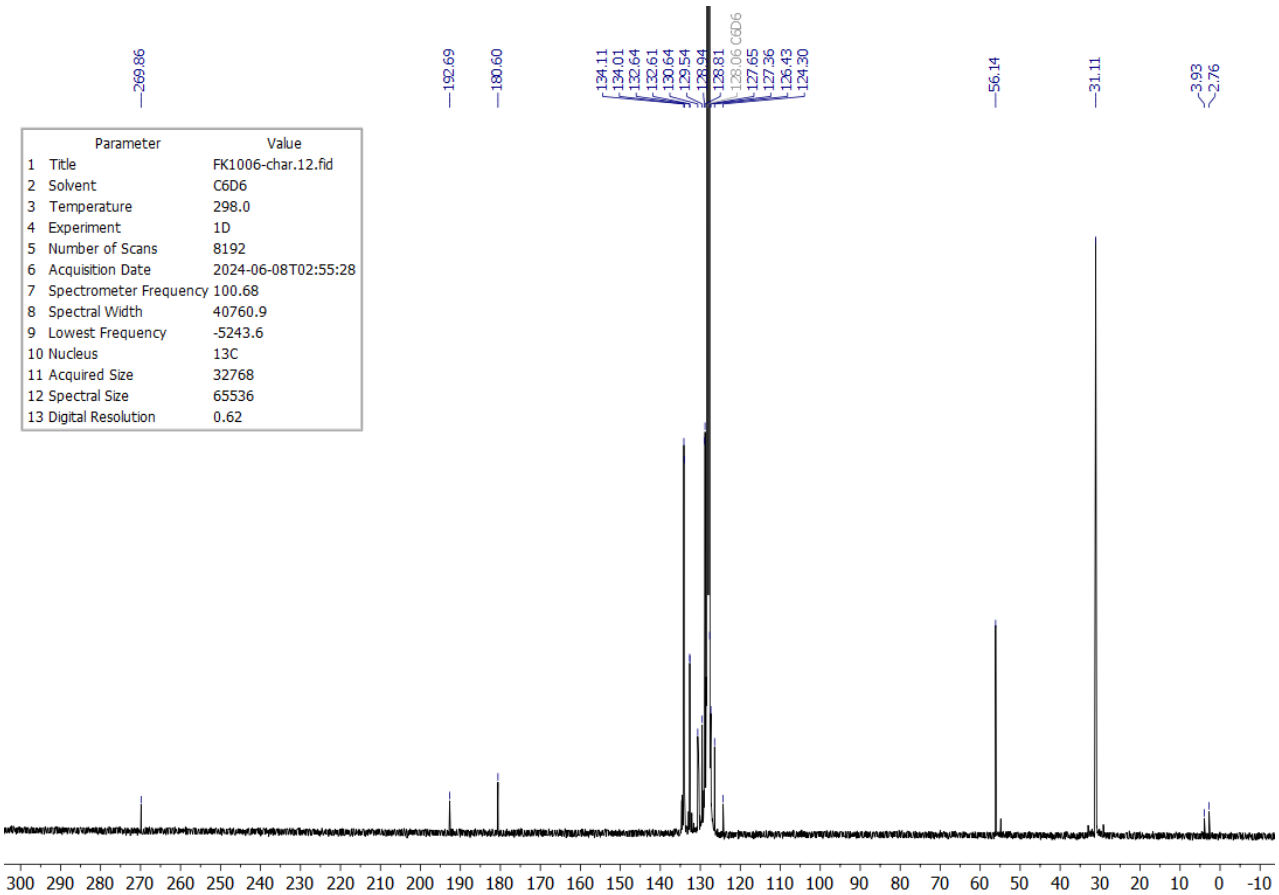


Figure S46. $^{13}C\{^{1}H\}$-NMR spectrum of **5$_{CN}$** in C_6D_6. The peak at 192.7 ppm corresponds to free CS_2.

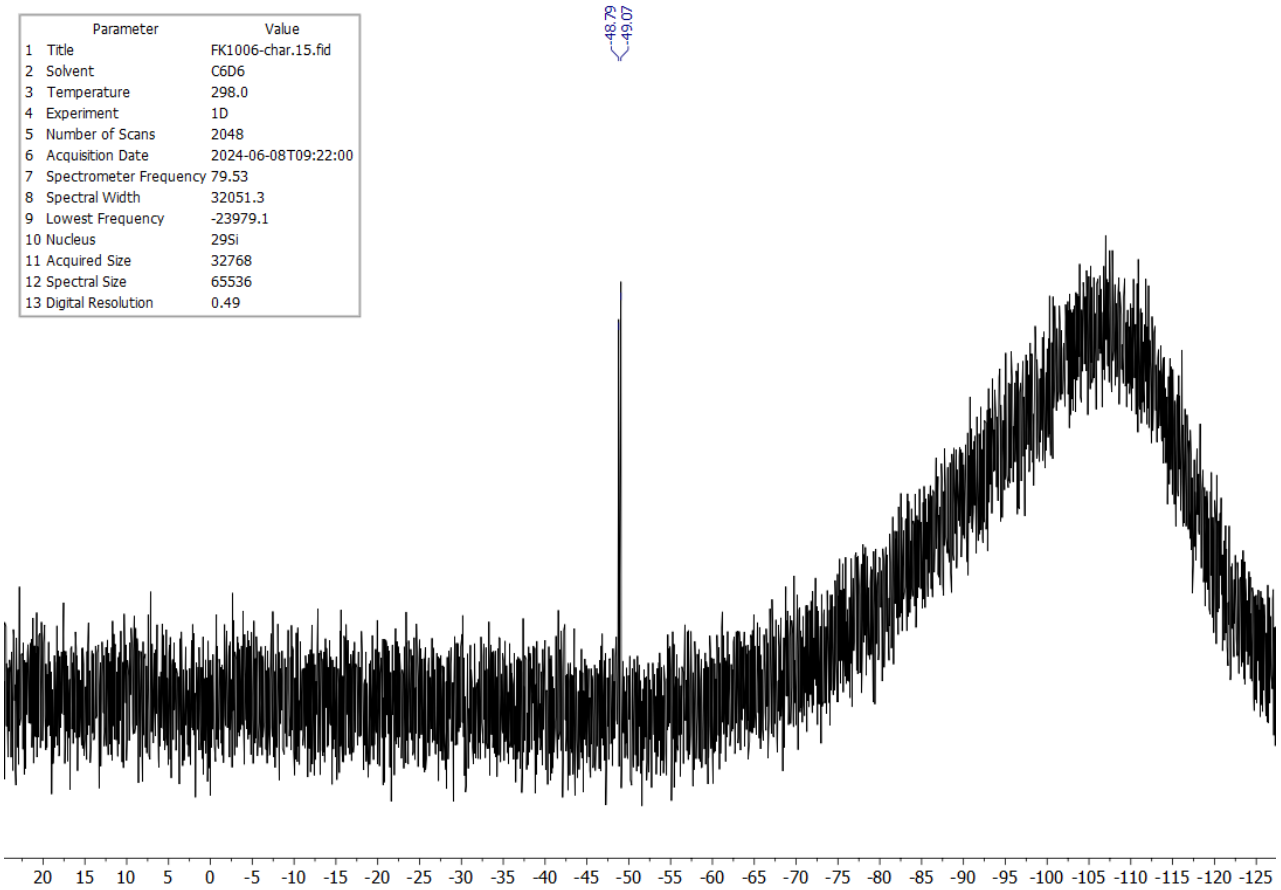


Figure S47. $^{29}Si\{^{1}H\}$-NMR spectrum of **5$_{CN}$** in C_6D_6.

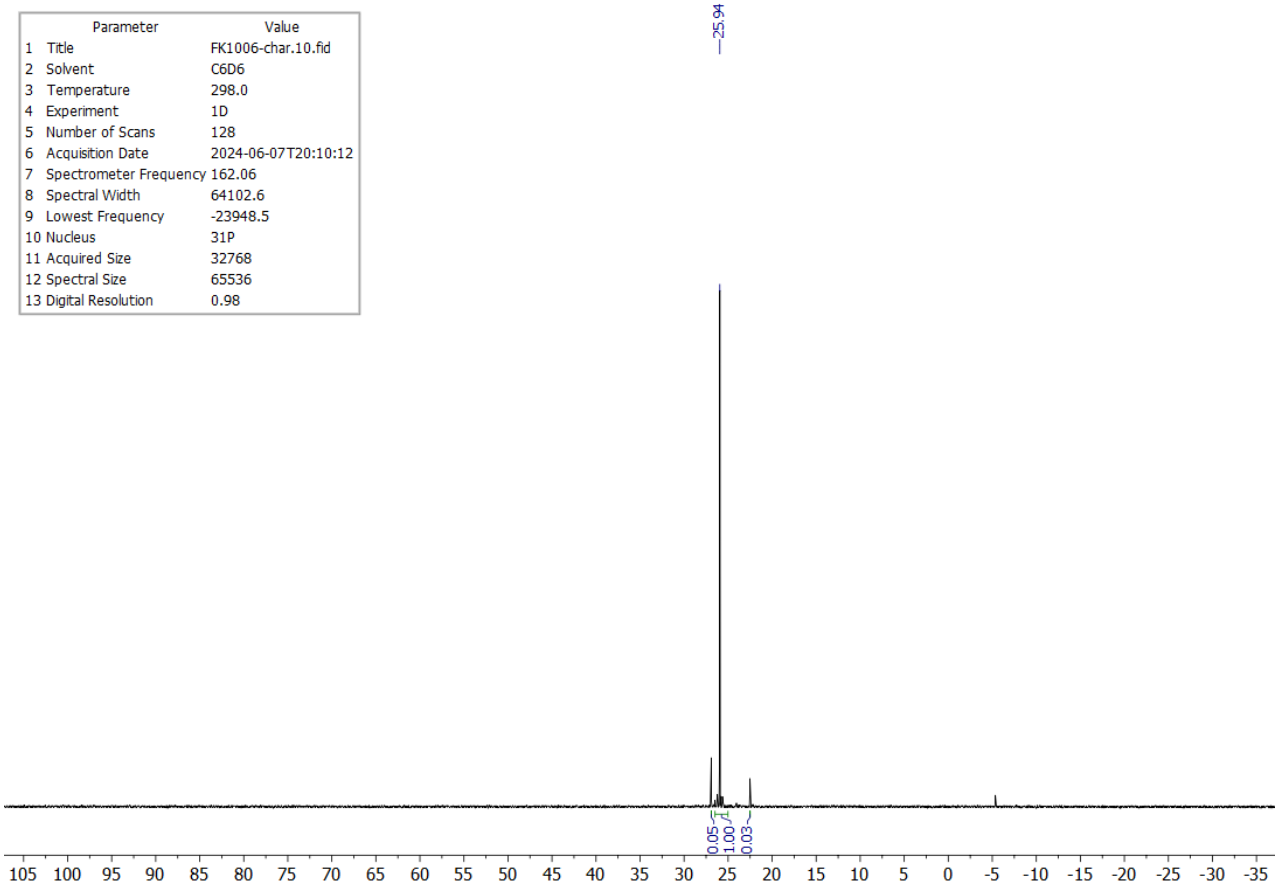


Figure S48. $^{31}P\{^{1}H\}$-NMR spectrum of **5$_{CN}$** in C_6D_6.

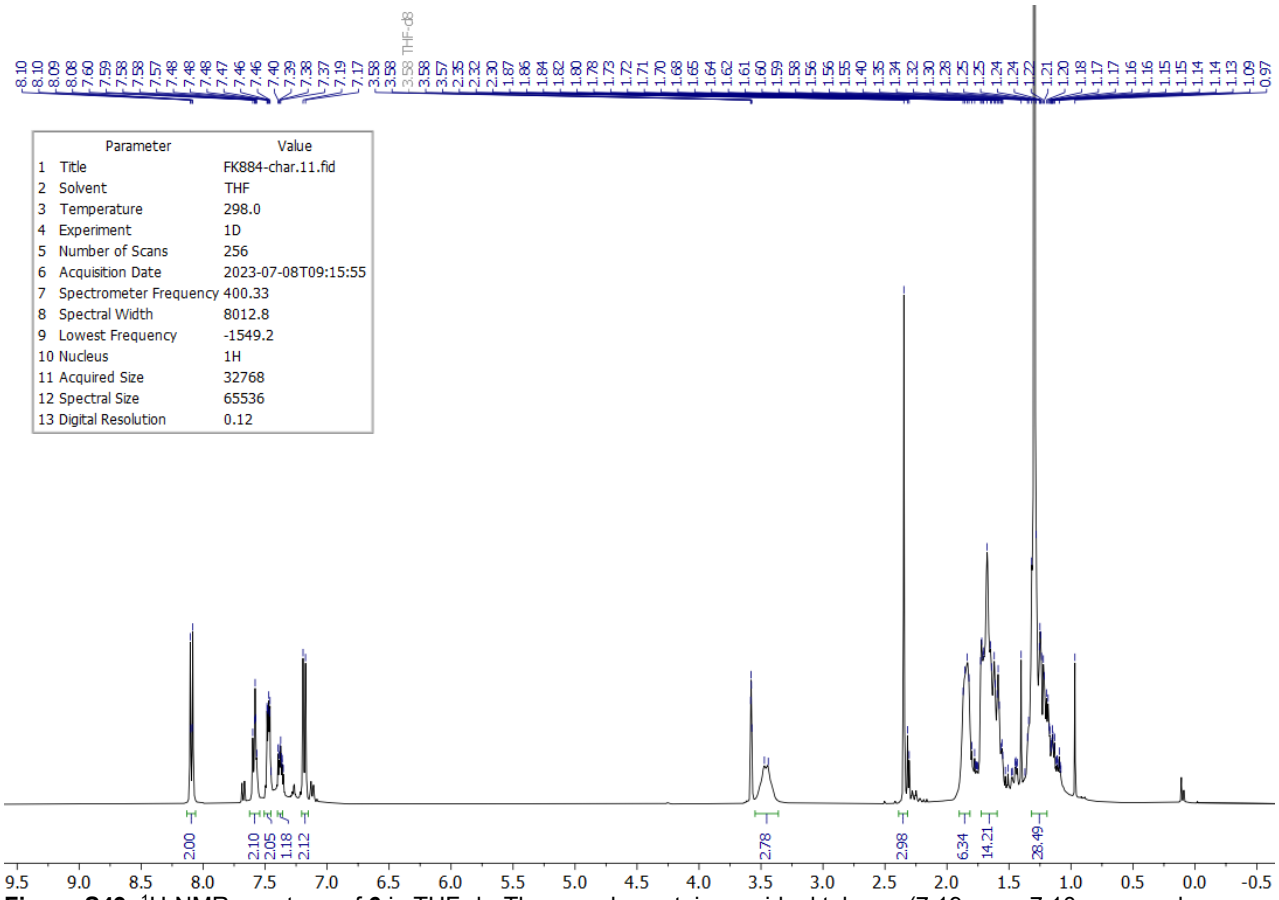


Figure S49. ^{1}H-NMR spectrum of **6** in THF-d_8. The sample contains residual toluene (7.19 ppm, 7.10 ppm, and 2.31 ppm).

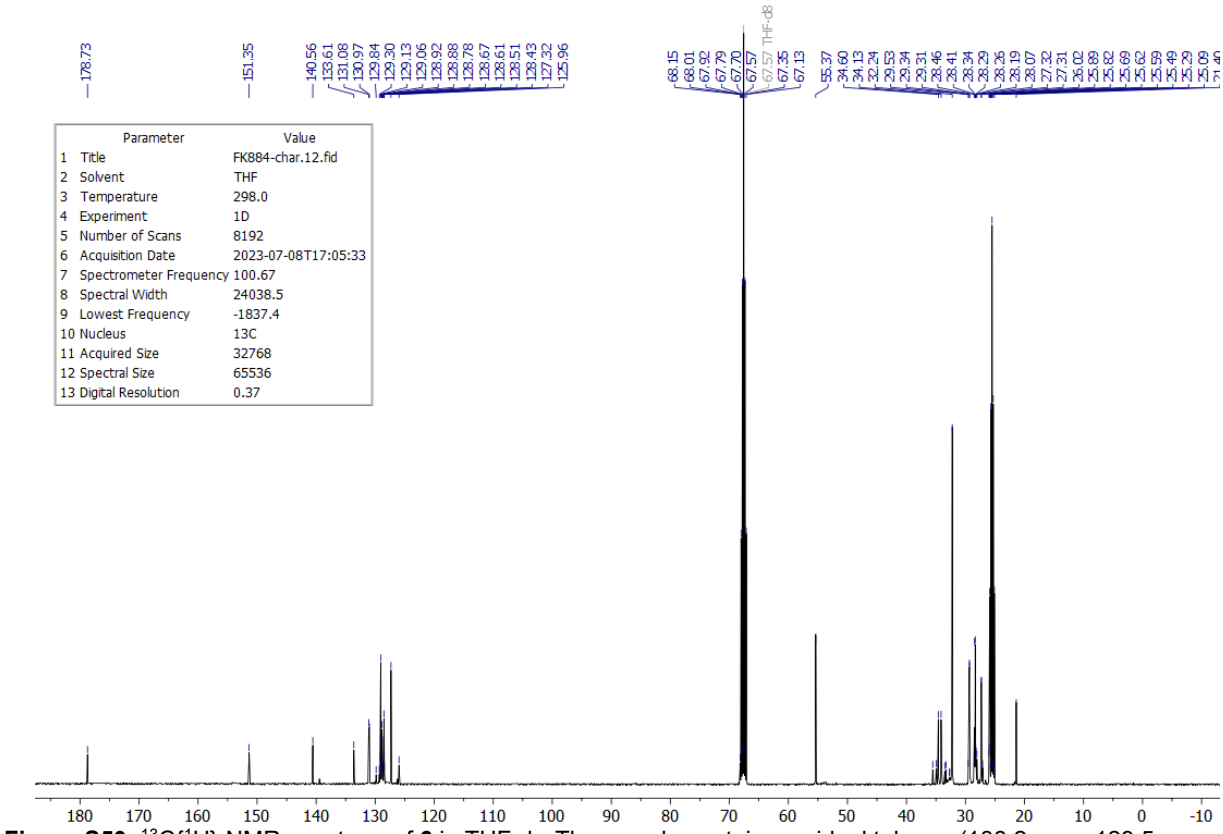
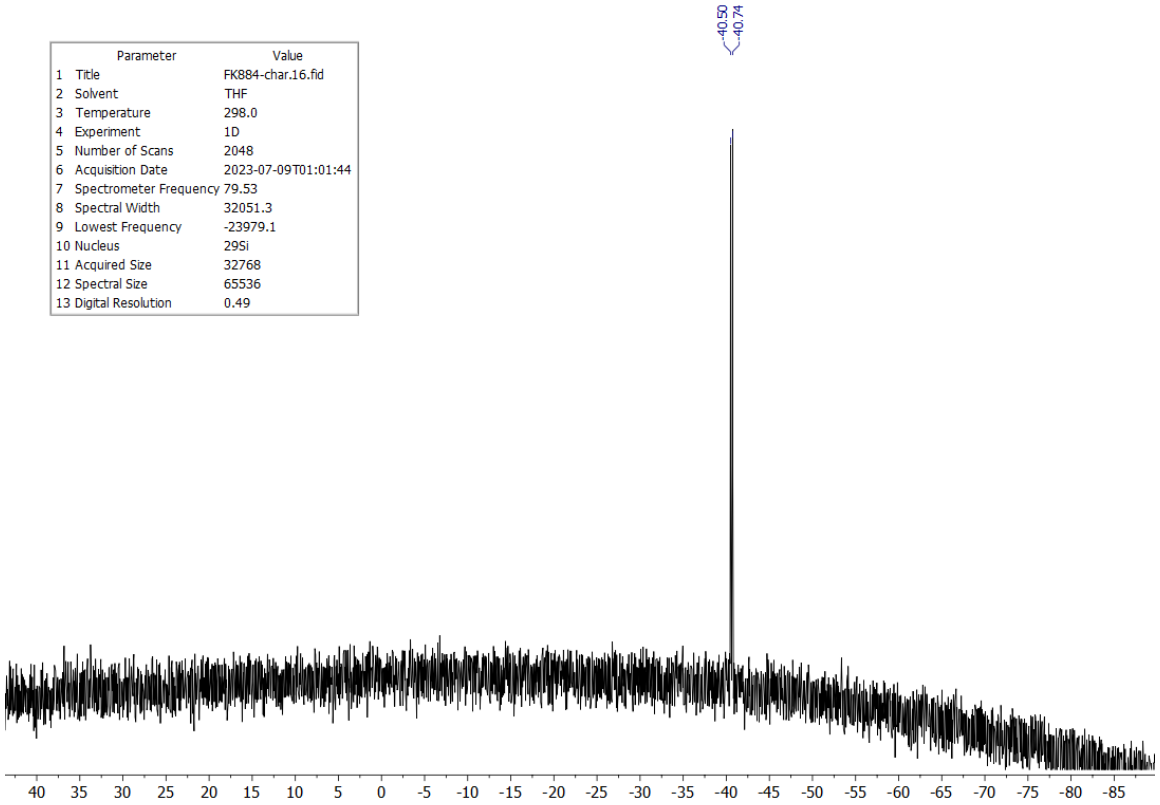
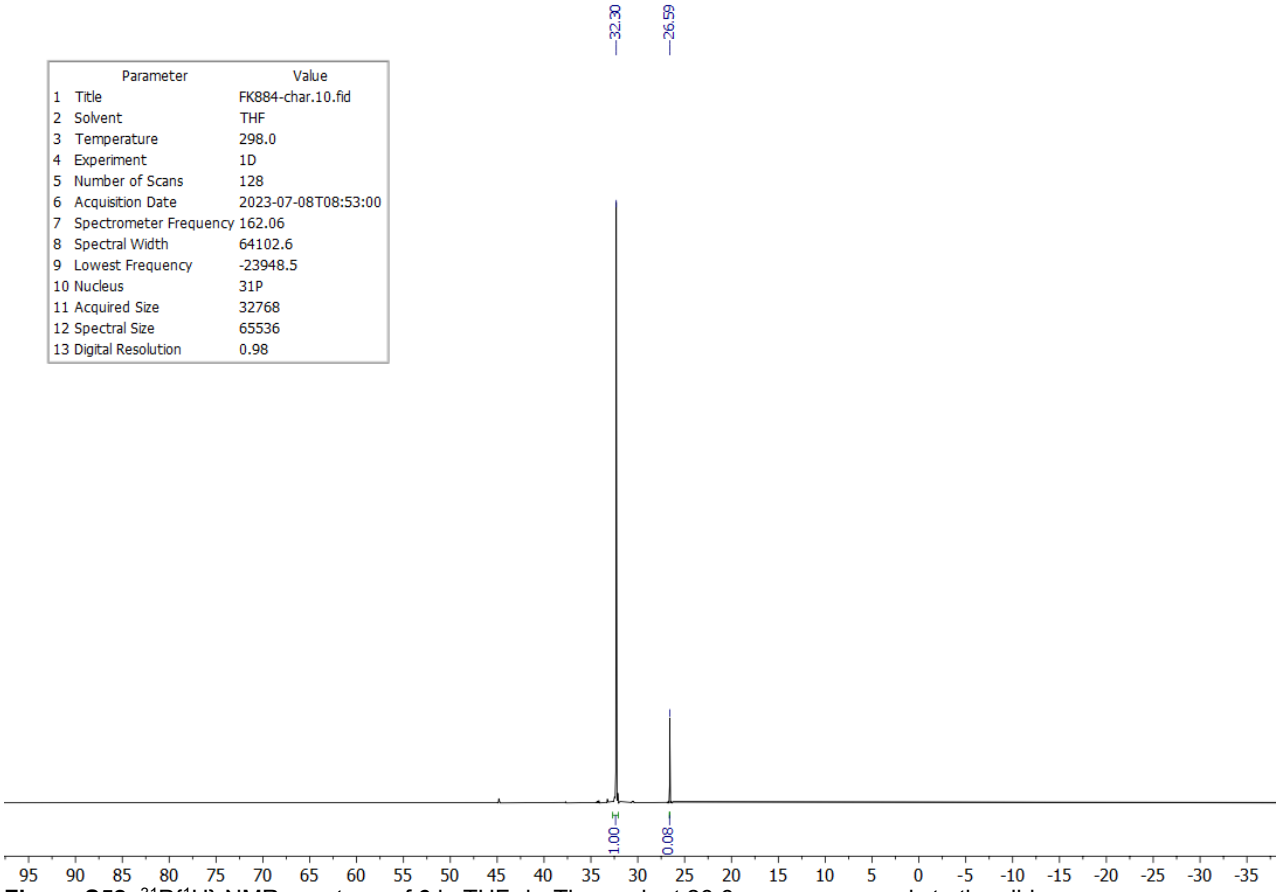


Figure S50. ^{13}C{^{1}H}-NMR spectrum of **6** in THF-d_8. The sample contains residual toluene (138.2 ppm, 129.5 ppm, 128.7 ppm, 125.8 ppm, and 21.3 ppm.)



Parameter	Value
1 Title	FK884-char.16.fid
2 Solvent	THF
3 Temperature	298.0
4 Experiment	1D
5 Number of Scans	2048
6 Acquisition Date	2023-07-09T01:01:44
7 Spectrometer Frequency	79.53
8 Spectral Width	32051.3
9 Lowest Frequency	-23979.1
10 Nucleus	29Si
11 Acquired Size	32768
12 Spectral Size	65536
13 Digital Resolution	0.49

Figure S51. $^{29}Si\{^{1}H\}$-NMR spectrum of **6** in THF-d_8.



Parameter	Value
1 Title	FK884-char.10.fid
2 Solvent	THF
3 Temperature	298.0
4 Experiment	1D
5 Number of Scans	128
6 Acquisition Date	2023-07-08T08:53:00
7 Spectrometer Frequency	162.06
8 Spectral Width	64102.6
9 Lowest Frequency	-23948.5
10 Nucleus	31P
11 Acquired Size	32768
12 Spectral Size	65536
13 Digital Resolution	0.98

Figure S52. $^{31}P\{^{1}H\}$-NMR spectrum of **6** in THF-d_8. The peak at 26.6 ppm corresponds to the ylide.

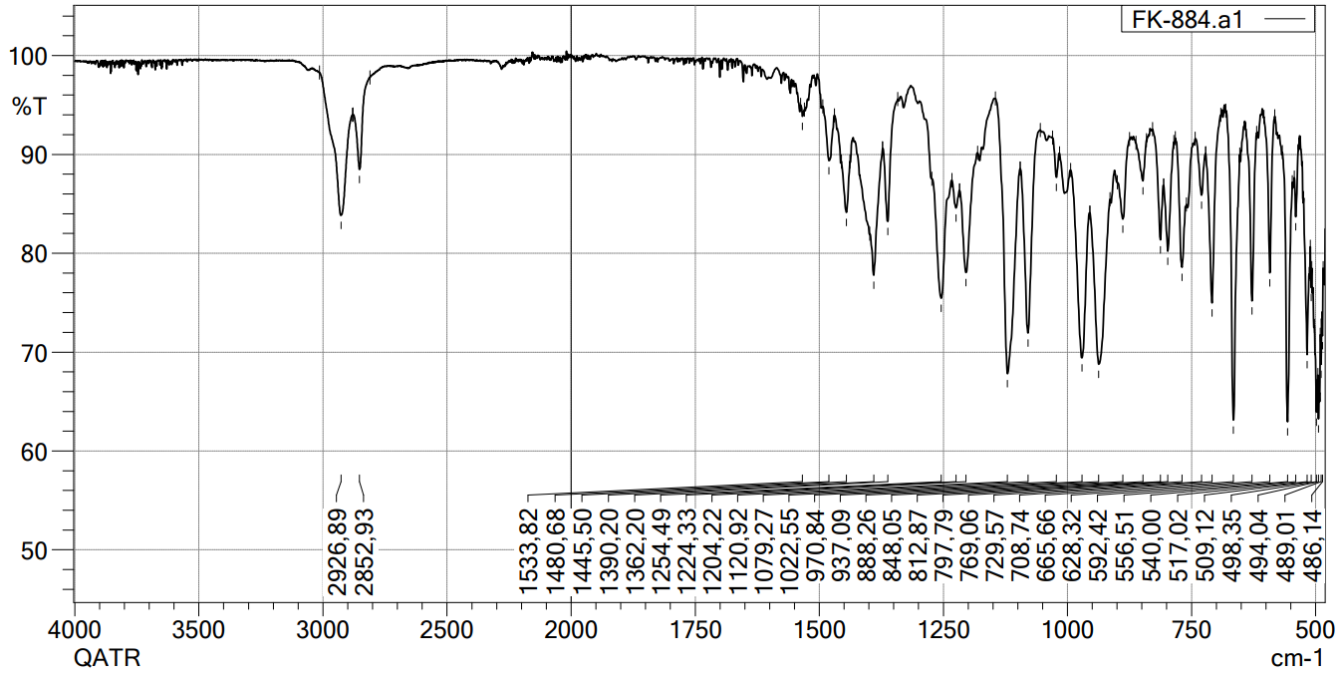


Figure S53. IR-Spectrum of solid **6**.

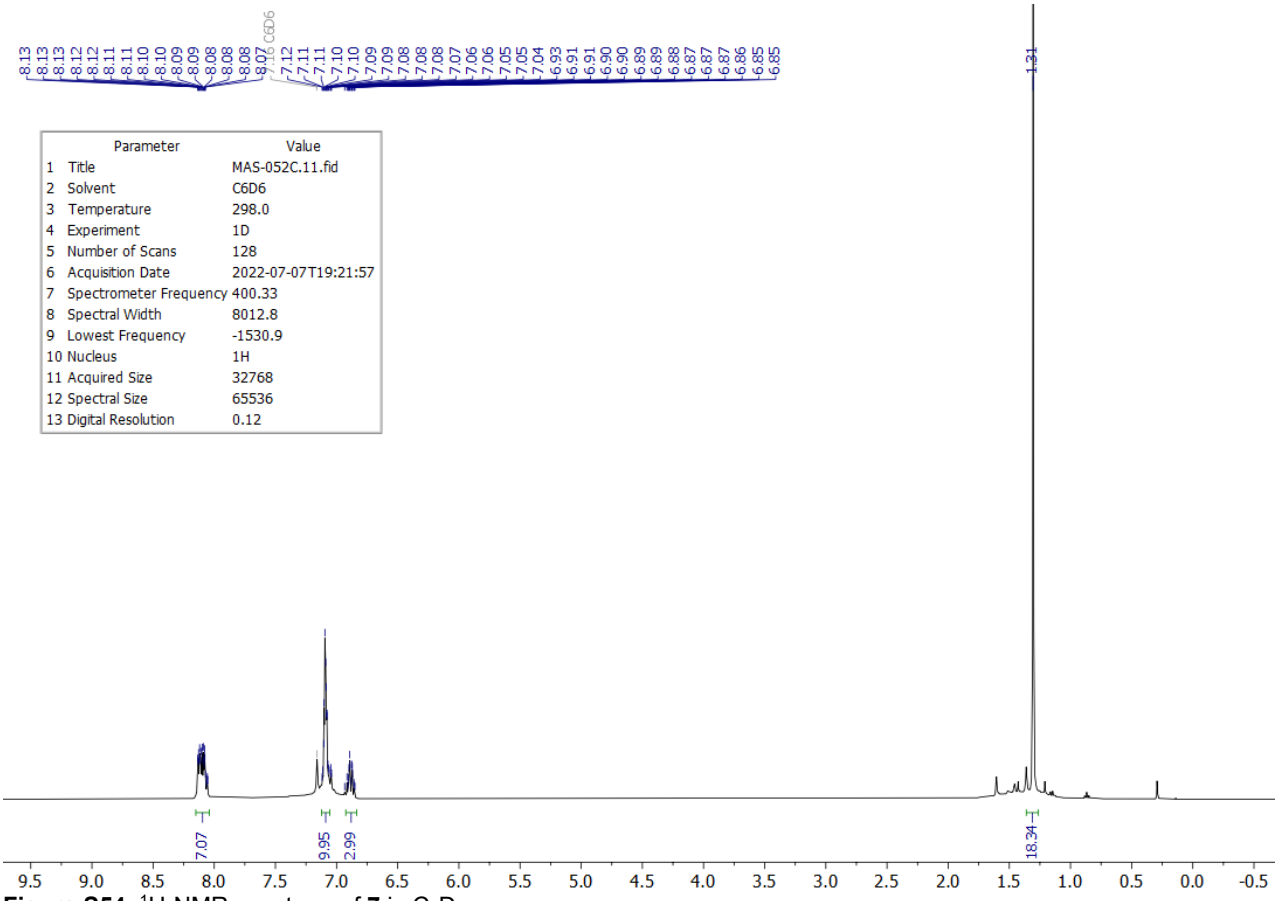


Figure S54. ^{1}H-NMR spectrum of **7** in C_6D_6.

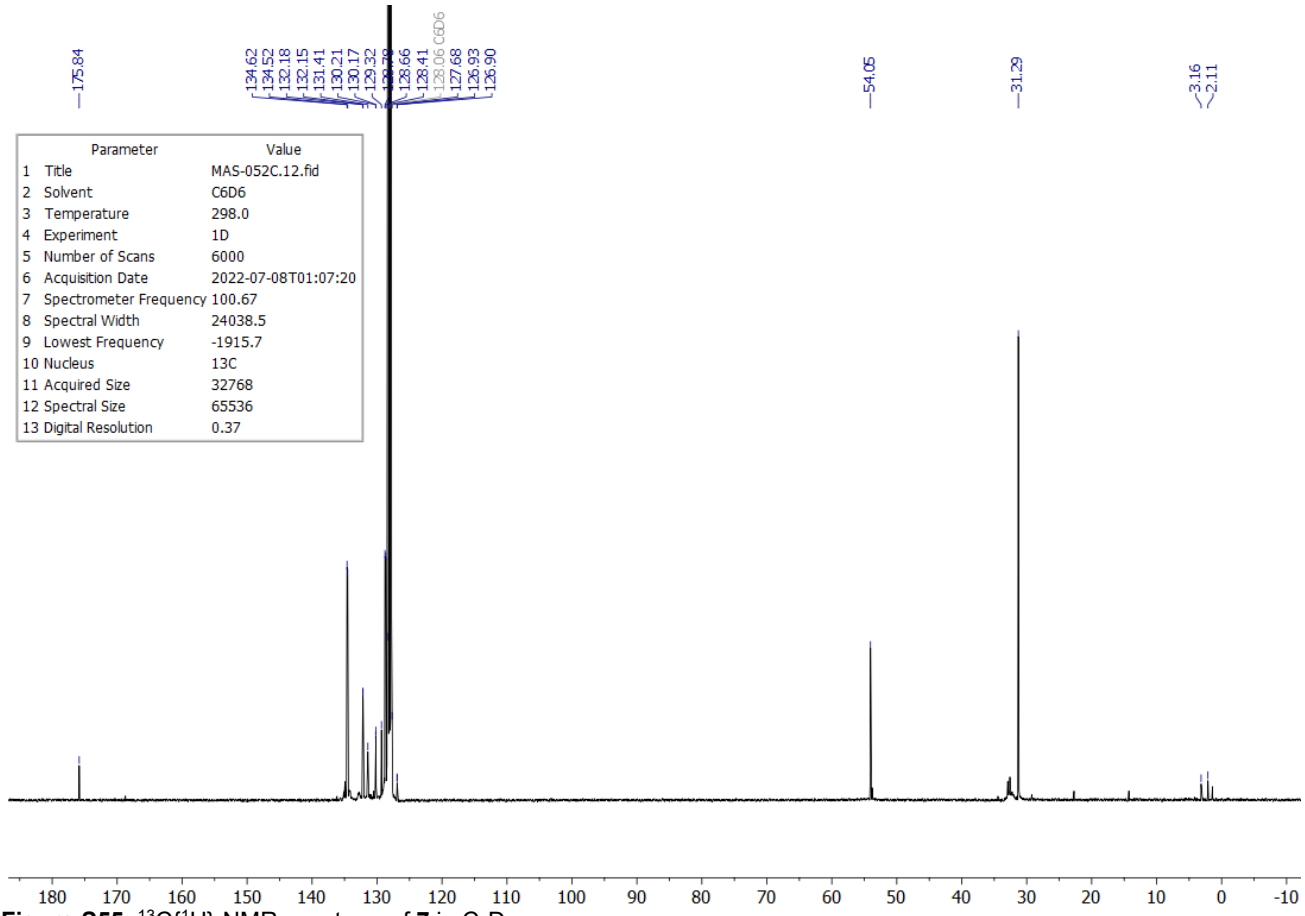


Figure S55. $^{13}C\{^{1}H\}$-NMR spectrum of **7** in C_6D_6.

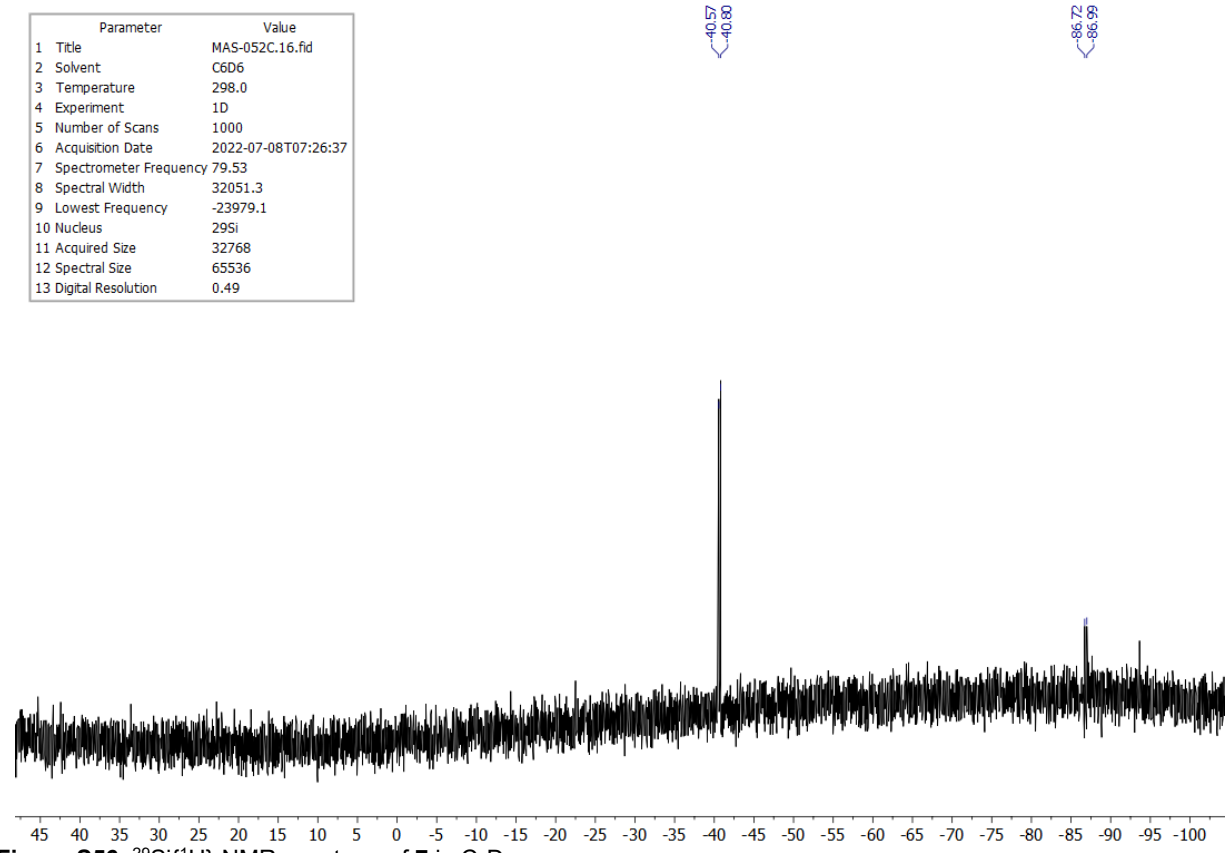


Figure S56. $^{29}Si\{^{1}H\}$-NMR spectrum of **7** in C_6D_6.

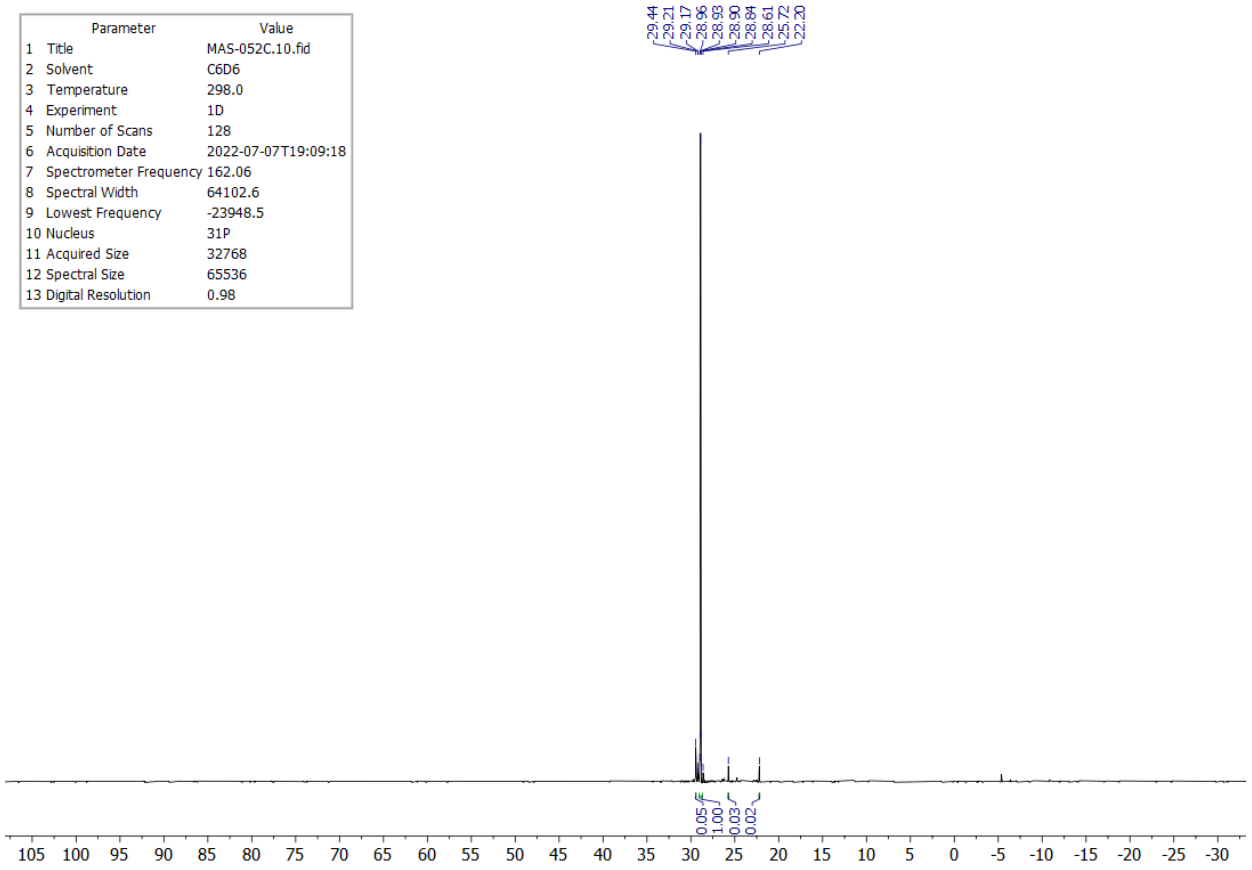


Figure S57. $^{31}P\{^{1}H\}$-NMR spectrum of **7** in C_6D_6.

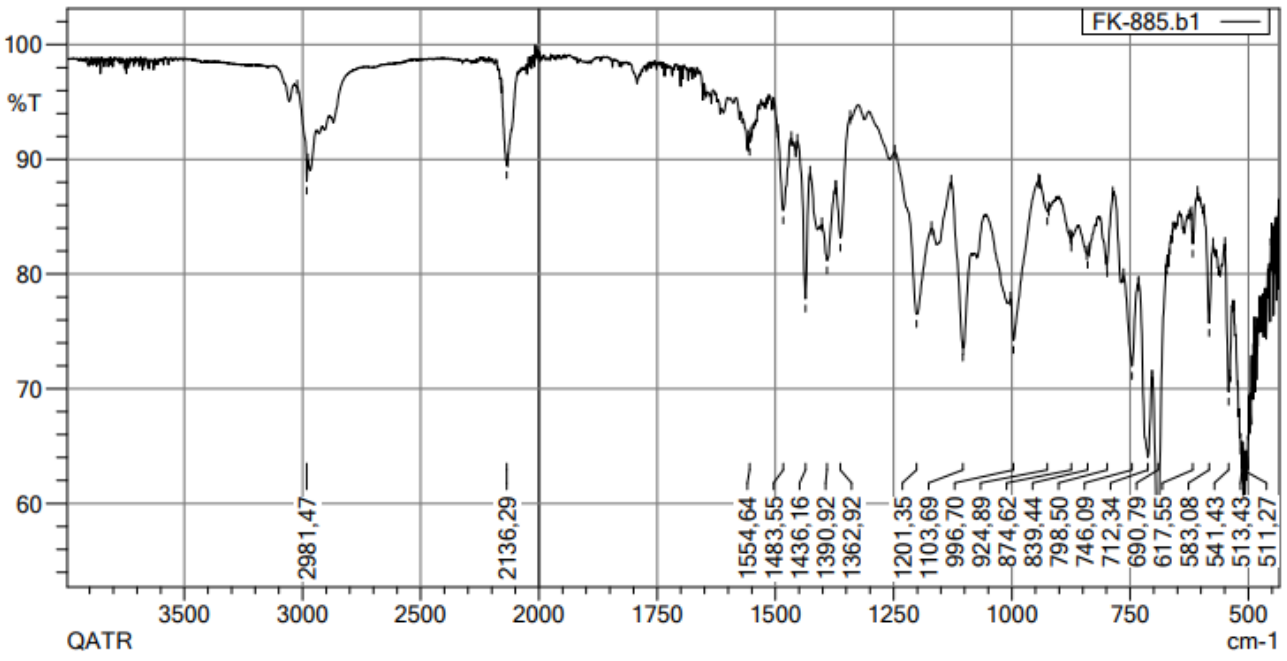


Figure S58. IR-spectrum of the dried reaction mixture of **7**.

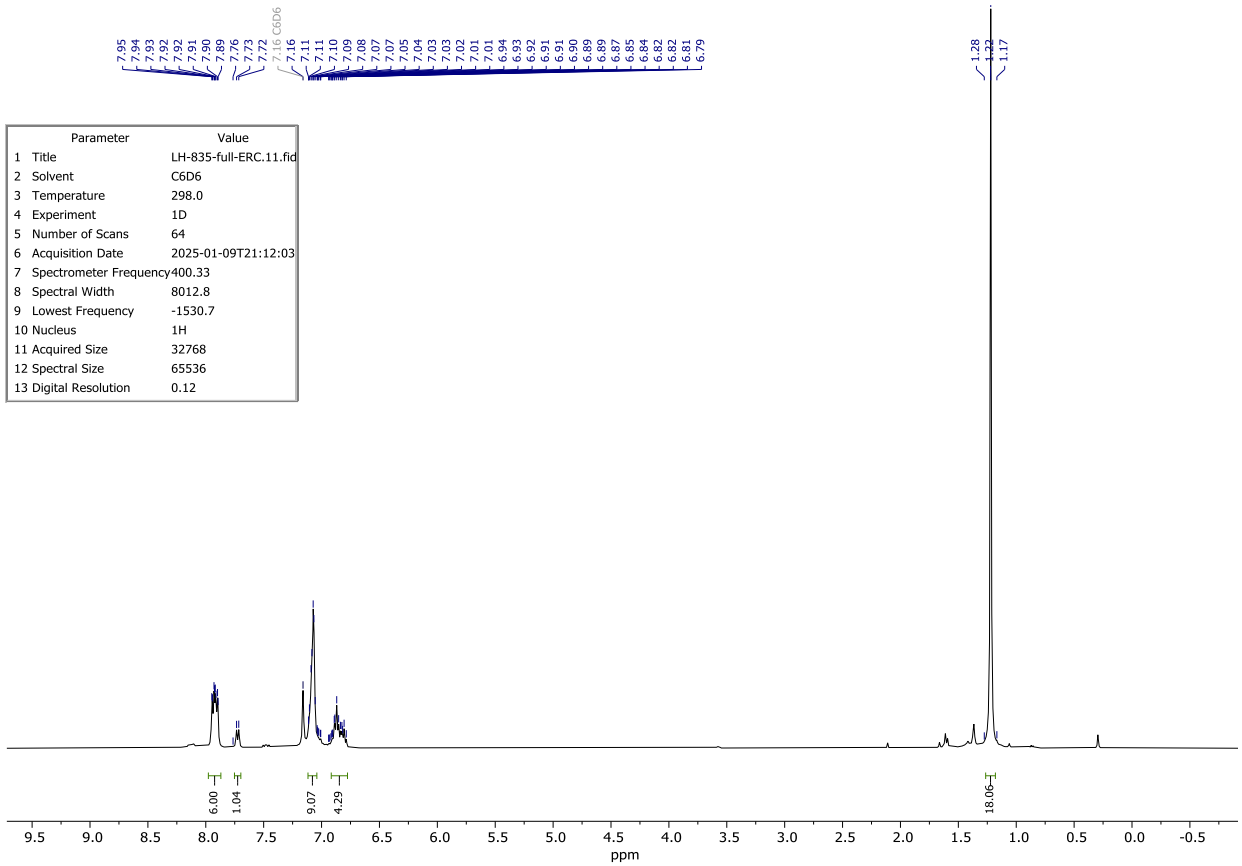


Figure S59. ^{1}H-NMR spectrum of **8** in C_6D_6.

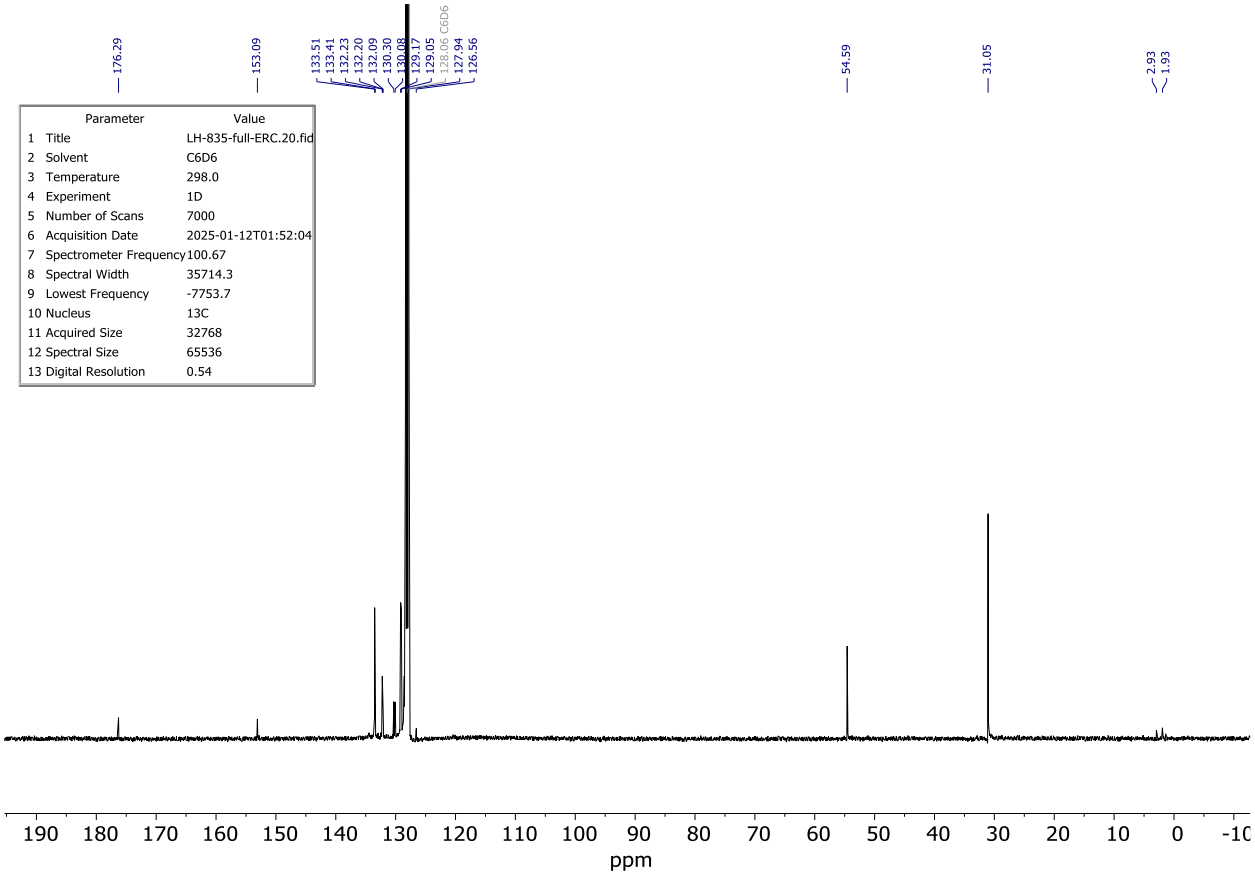


Figure S60: ^{13}C{^{1}H}-NMR spectrum of **8** in C_6D_6.

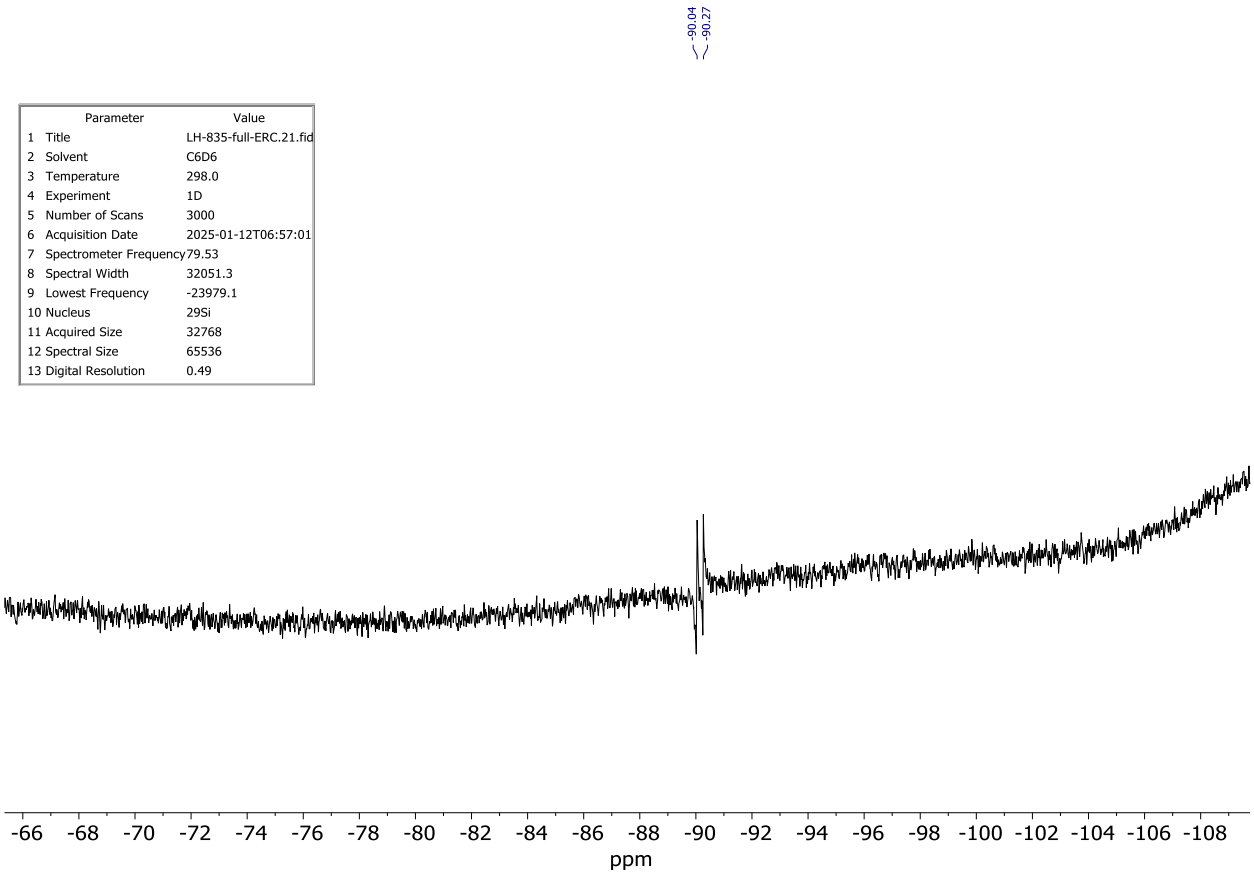


Figure S61: $^{29}Si\{^{1}H\}$-NMR spectrum of **8** in C_6D_6.

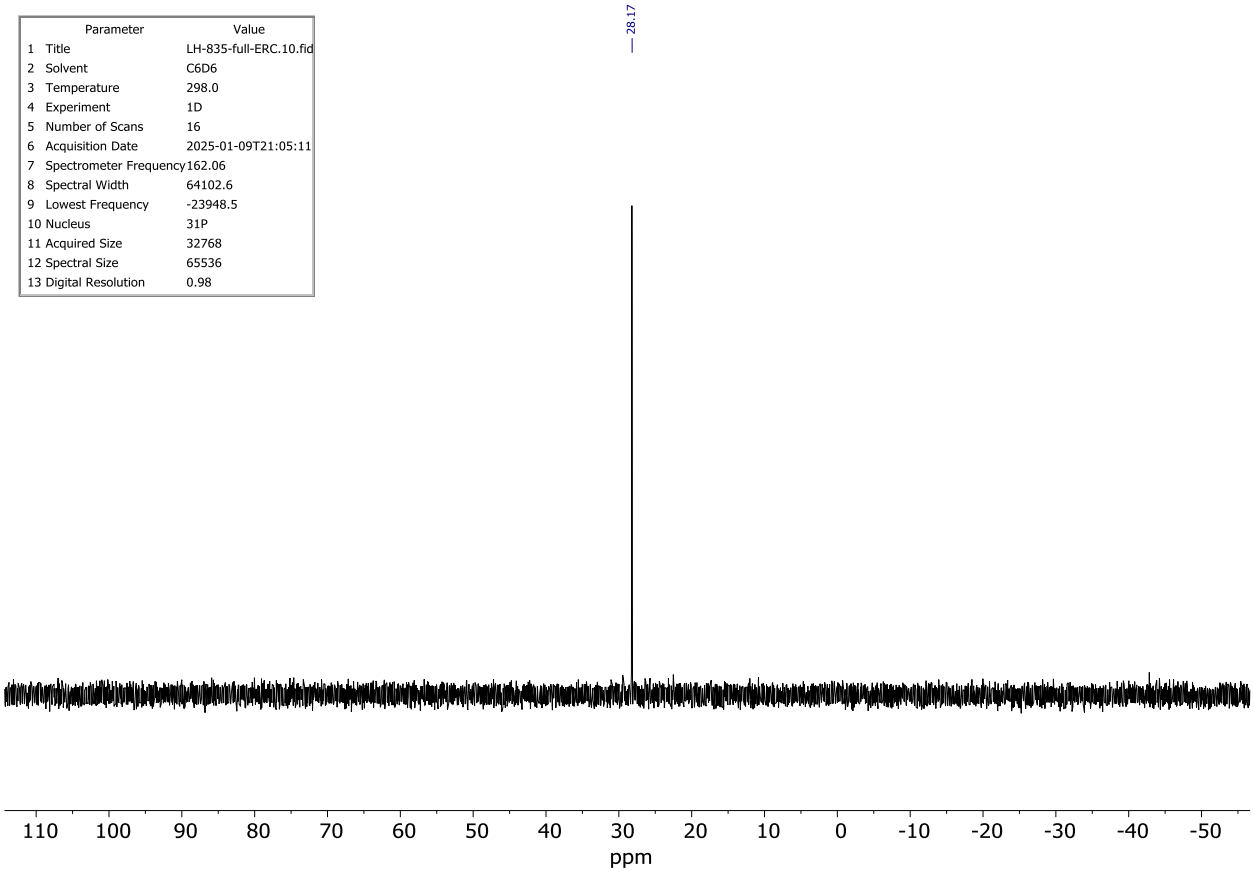


Figure S62: $^{31}P\{^{1}H\}$-NMR spectrum of **8** in C_6D_6.

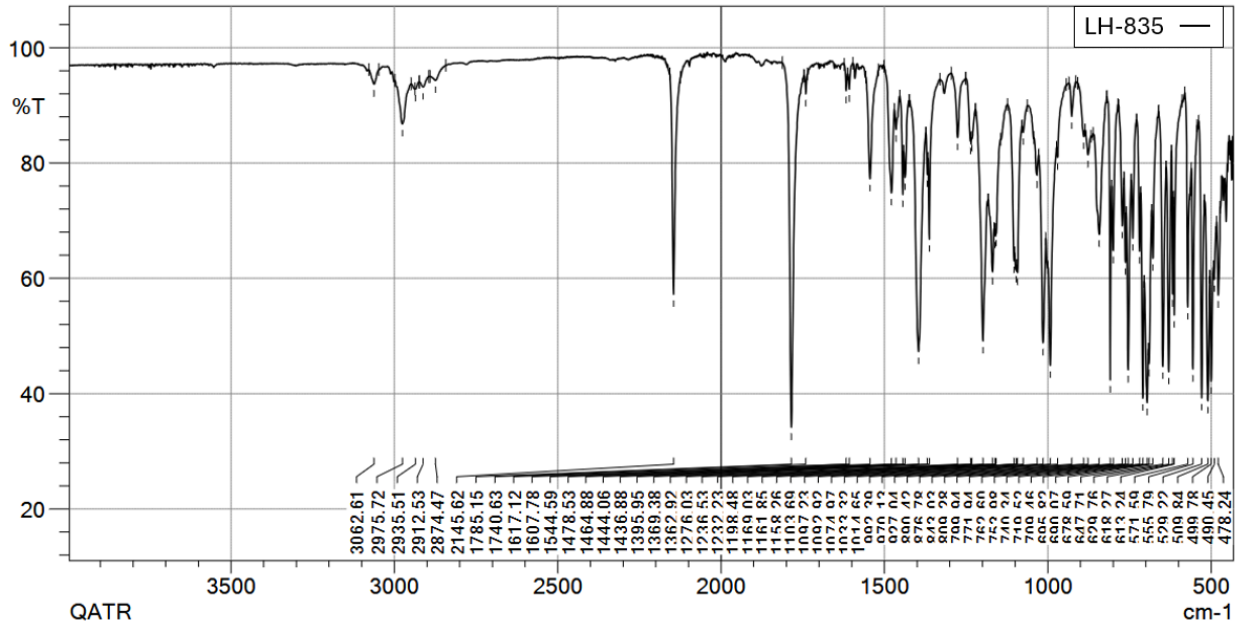


Figure S63: IR spectrum of solid **8**.

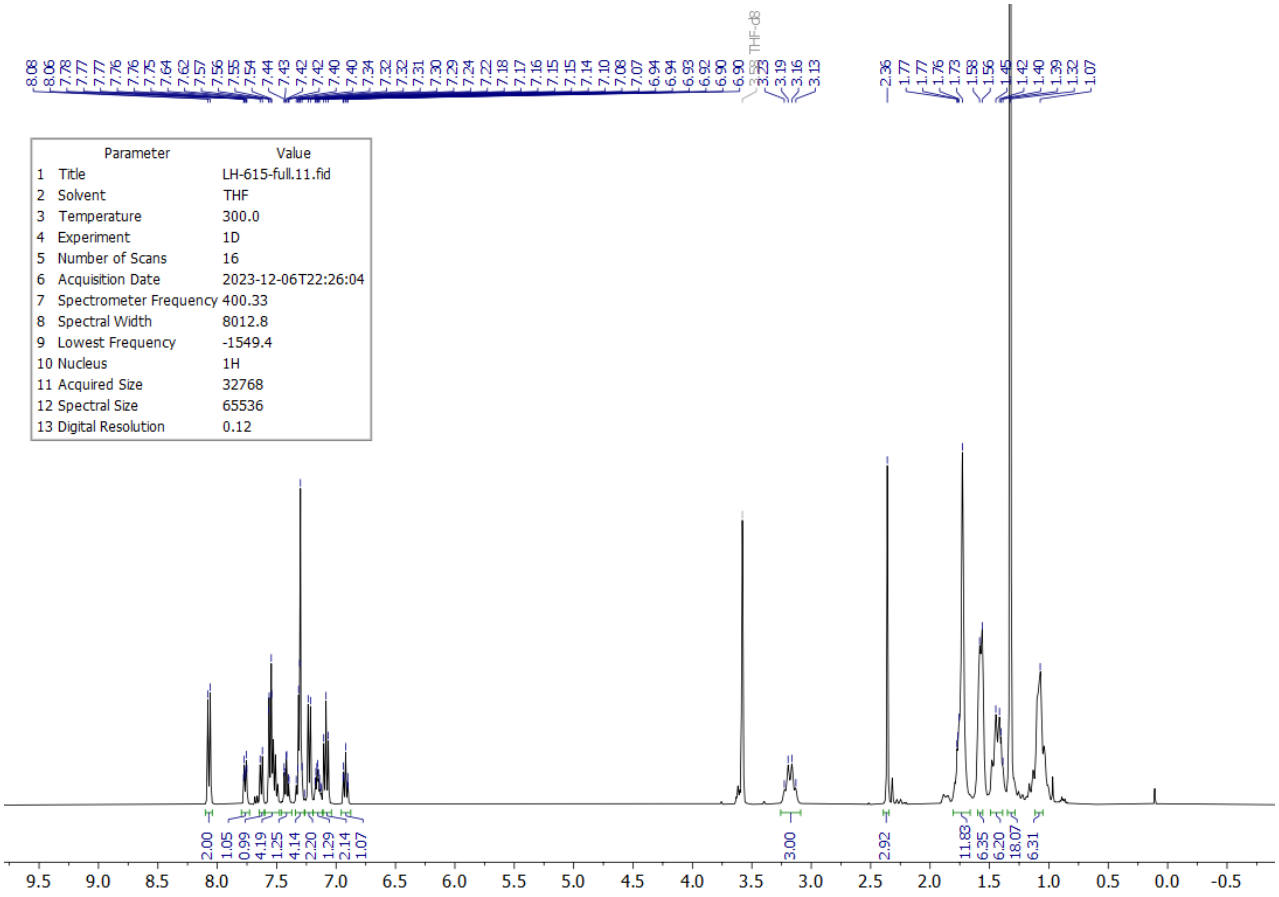


Figure S64: ^{1}H-NMR spectrum of $\mathbf{9_{Ts}}$ in THF-d_8.

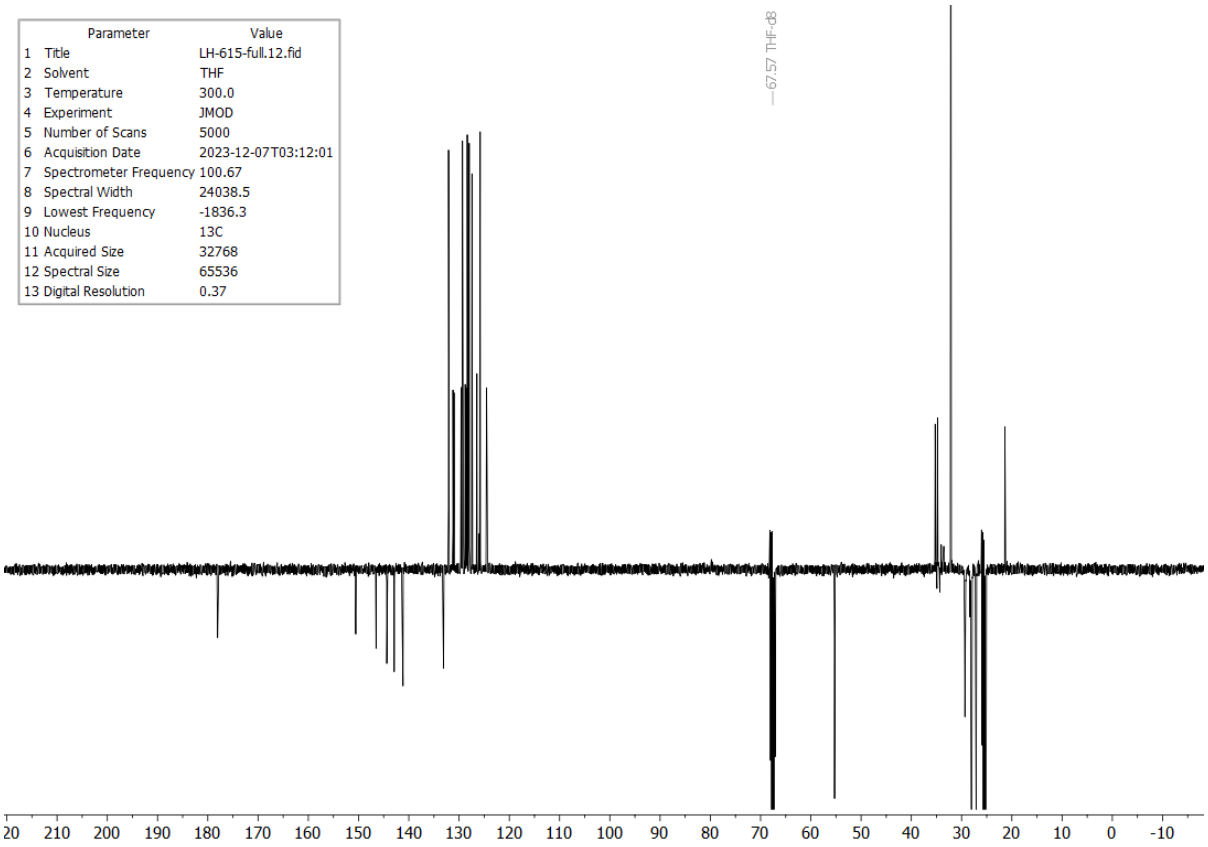


Figure S65: $^{13}C\{^{1}H\}$-APT-NMR spectrum of $\mathbf{9_{Ts}}$ in THF-d_8.

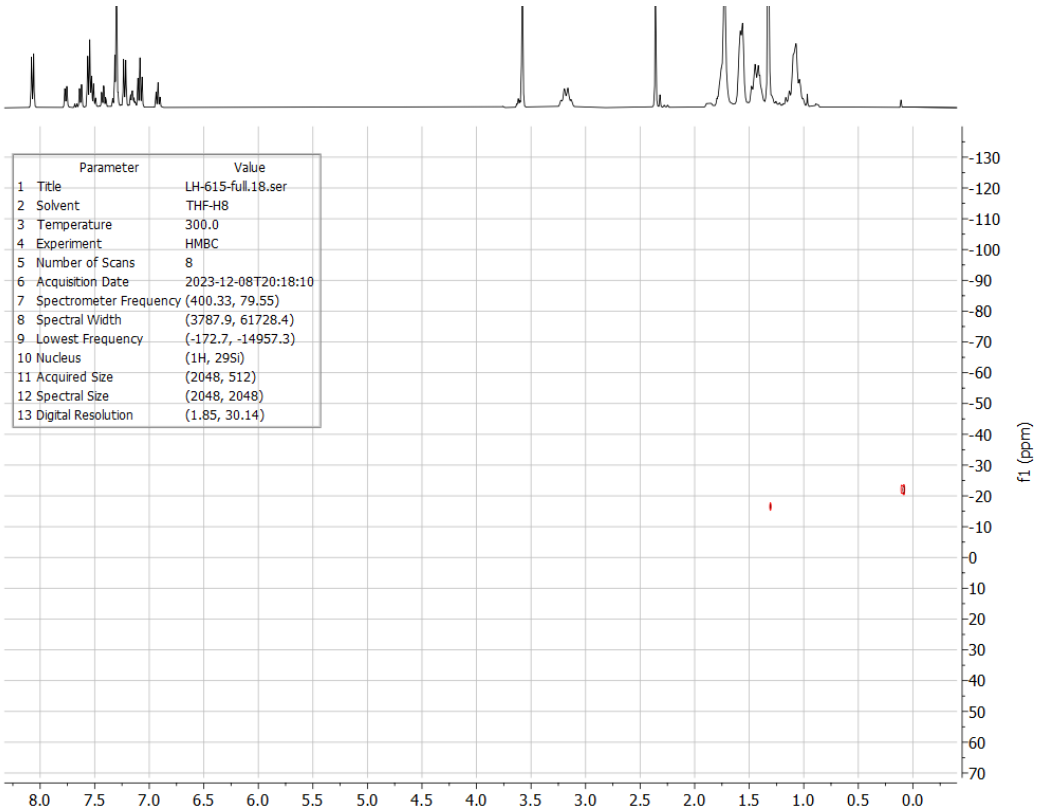


Figure S66: ^{1}H-^{29}Si-HMBC-NMR spectrum of $\mathbf{9_{Ts}}$ in THF-d_8. The cross-peak at (0.11/-22.1) ppm corresponds to residual silicon grease.

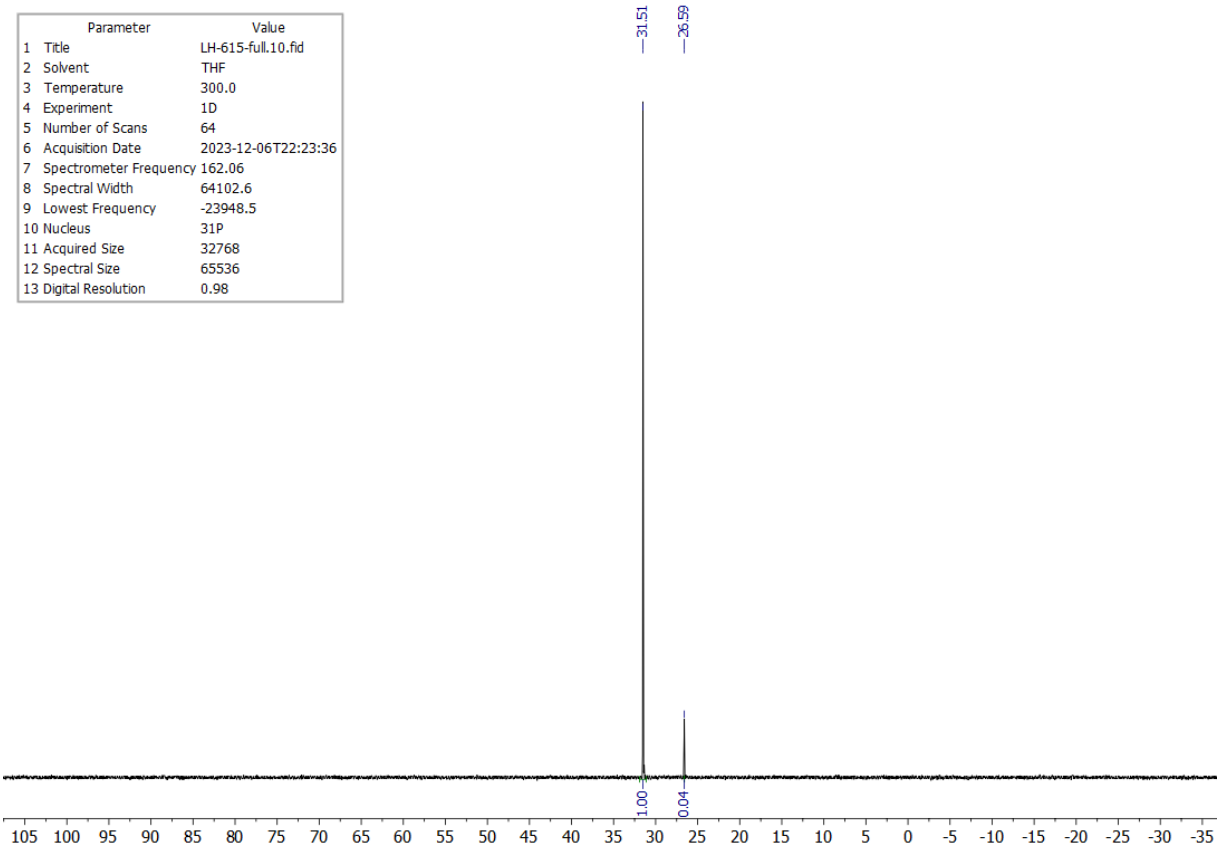


Figure S67: $^{31}P\{^{1}H\}$-NMR spectrum of $\mathbf{9_{Ts}}$ in THF-d_8. The peak at 26.6 ppm corresponds to free ylide.

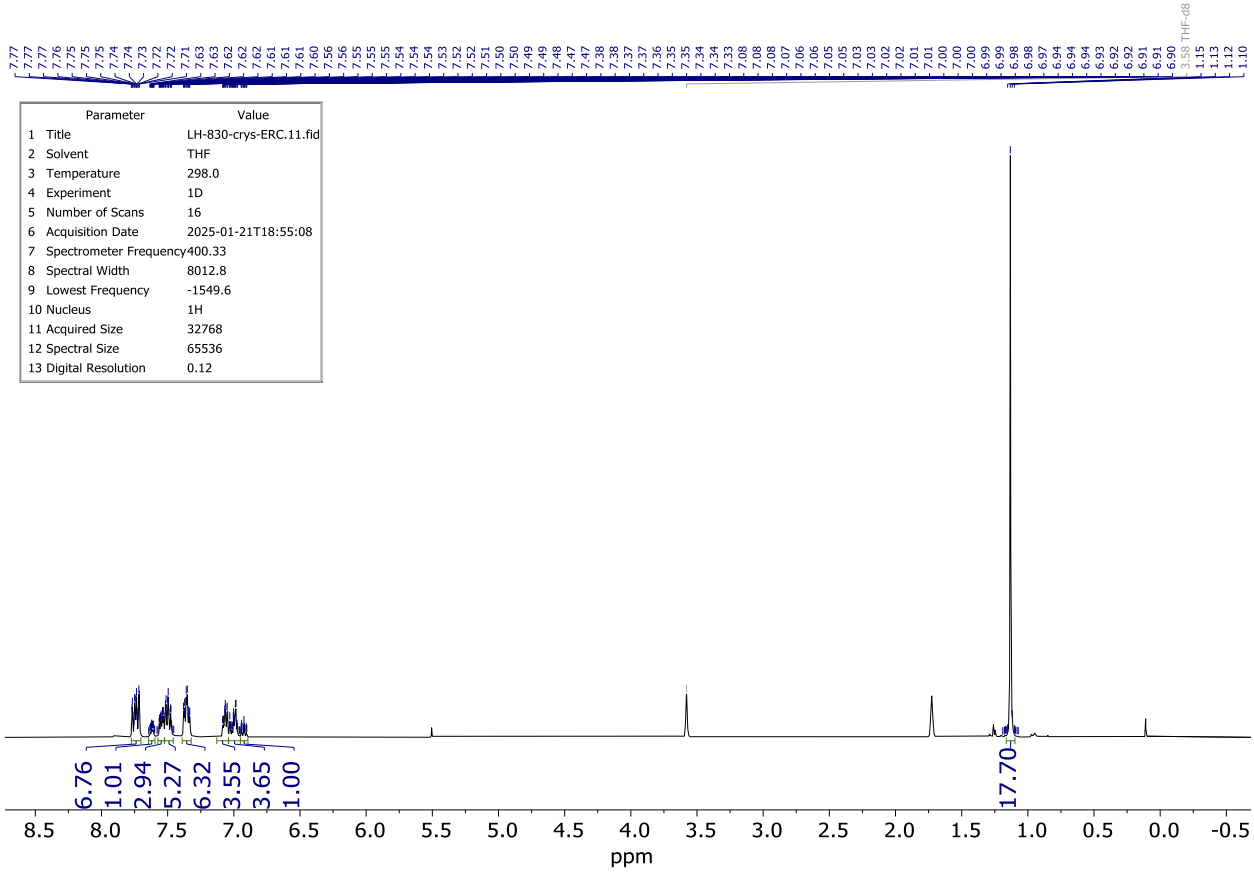


Figure S68: ^{1}H-NMR spectrum of $\mathbf{9_{CN}}$ in THF-d_8.

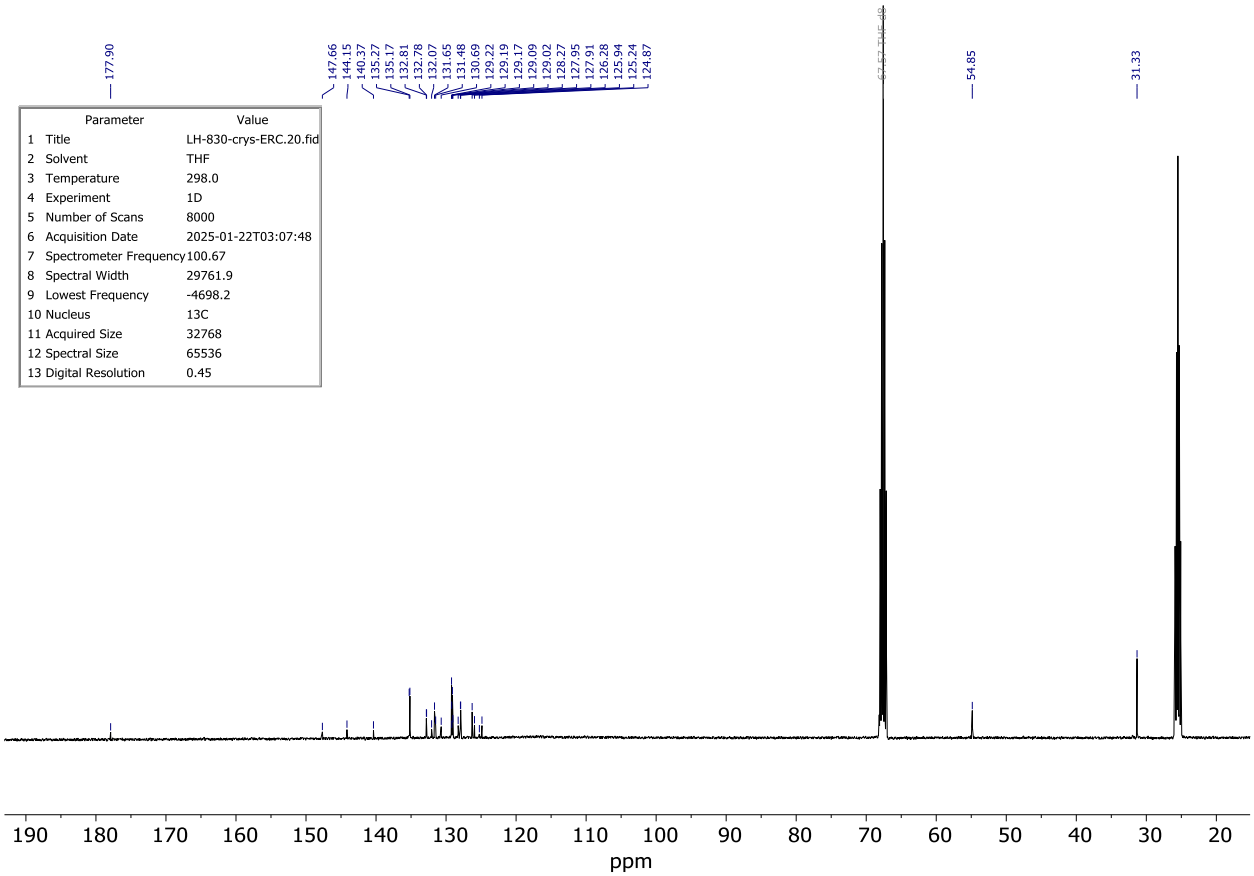


Figure S69: $^{13}C\{^{1}H\}$-NMR spectrum of **9_{CN}** in THF-d_8.

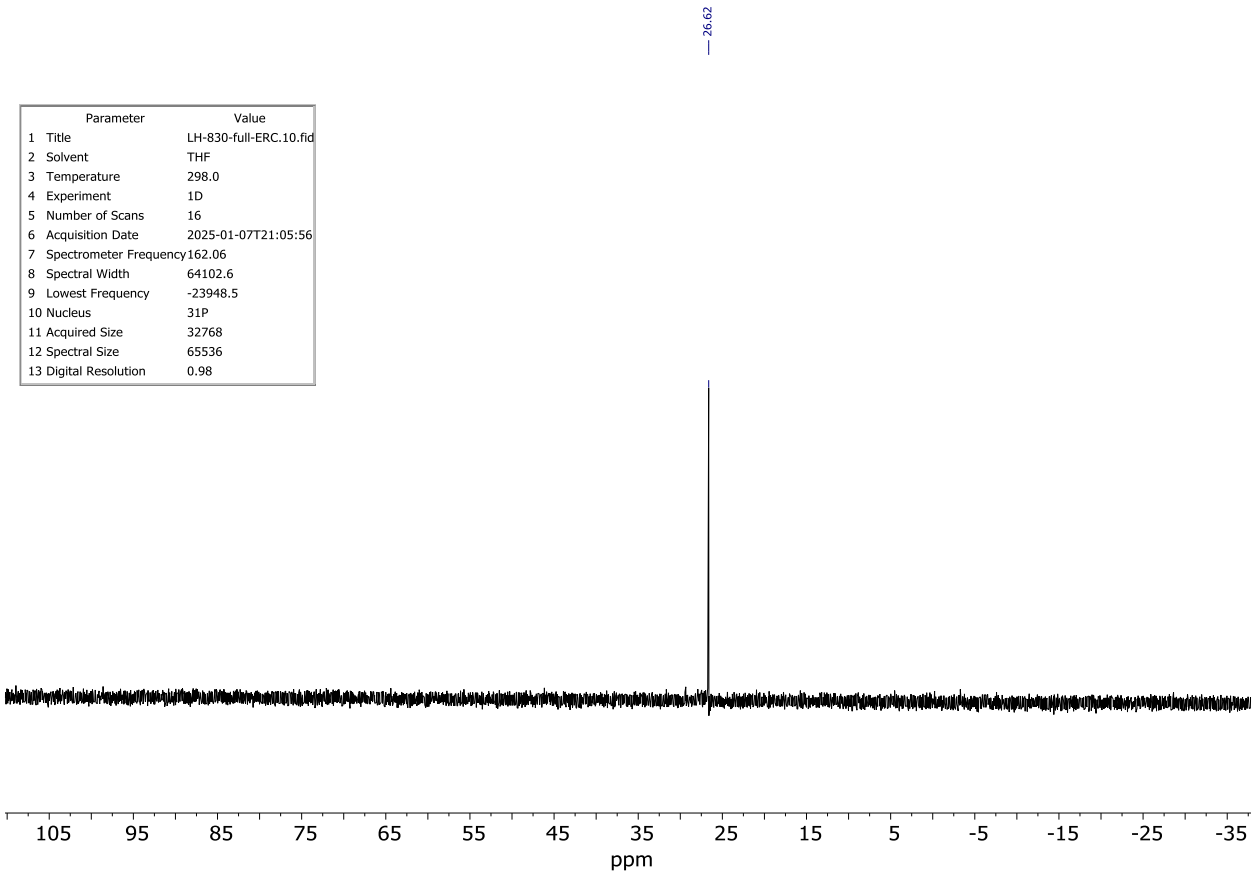


Figure S70: $^{31}P\{^{1}H\}$-NMR spectrum of **9_{CN}** in THF-d_8.

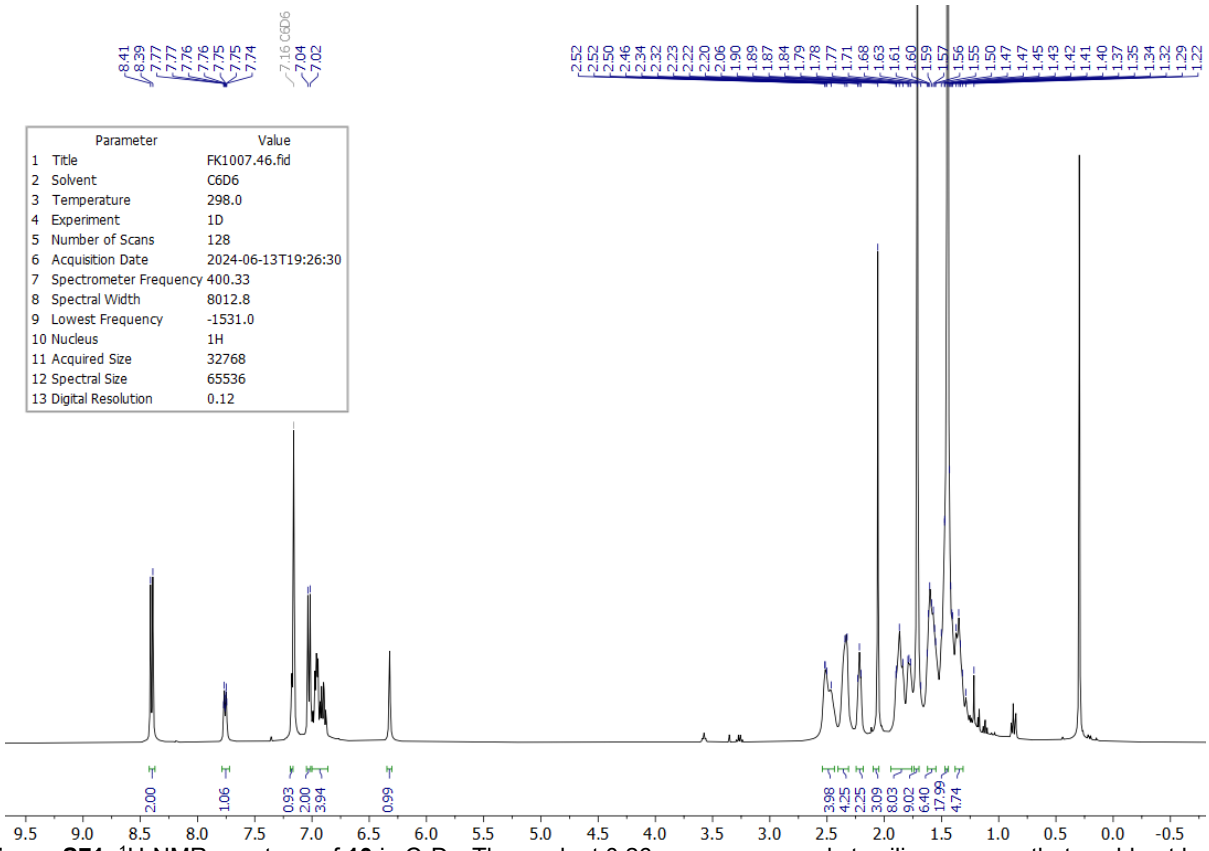


Figure S71. ^{1}H-NMR spectrum of **10** in C_6D_5- The peak at 0.26 ppm corresponds to silicon grease that could not be removed due to similar solubility.

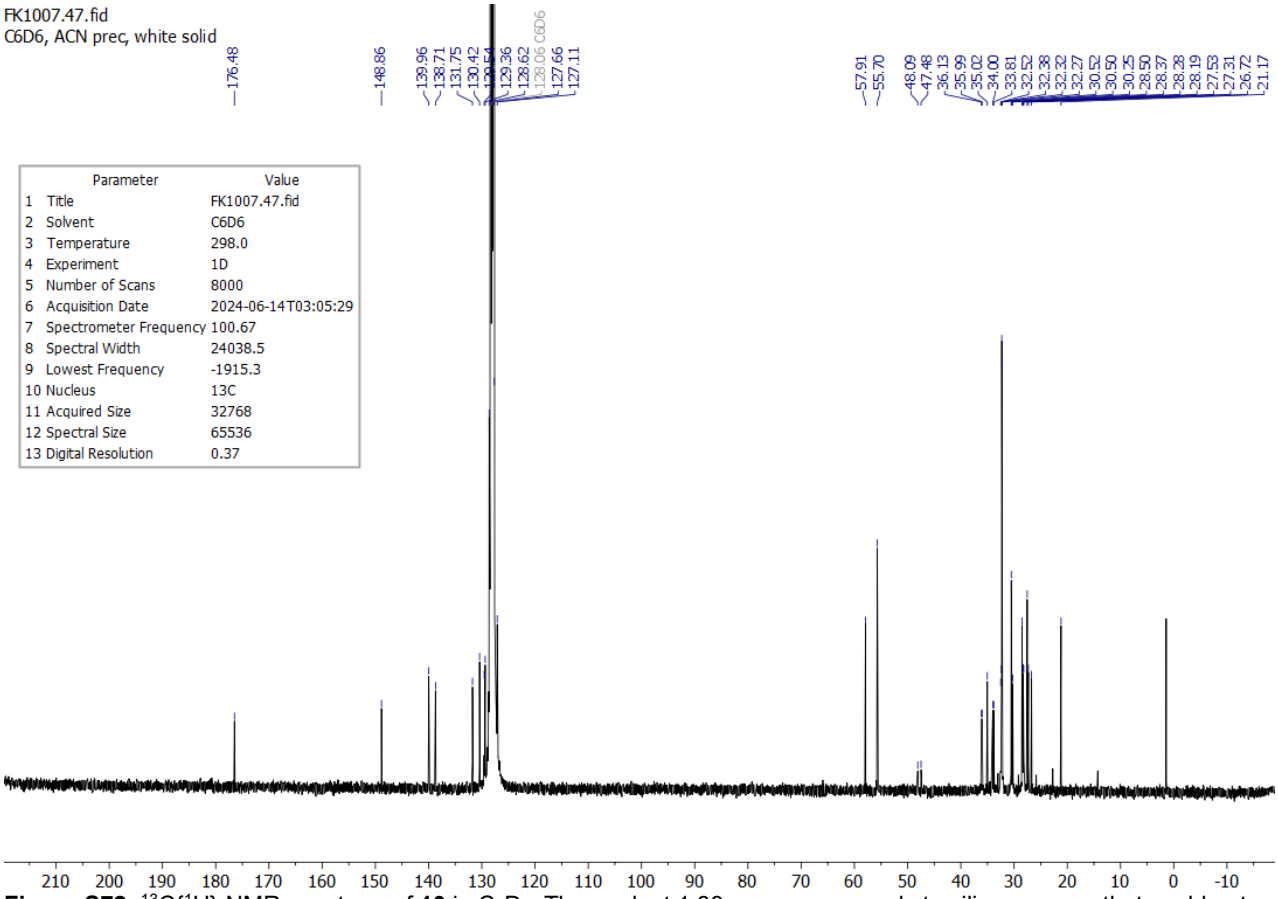


Figure S72. $^{13}C\{^{1}H\}$-NMR spectrum of **10** in C_6D_6. The peak at 1.38 ppm corresponds to silicon grease that could not be removed due to similar solubility.

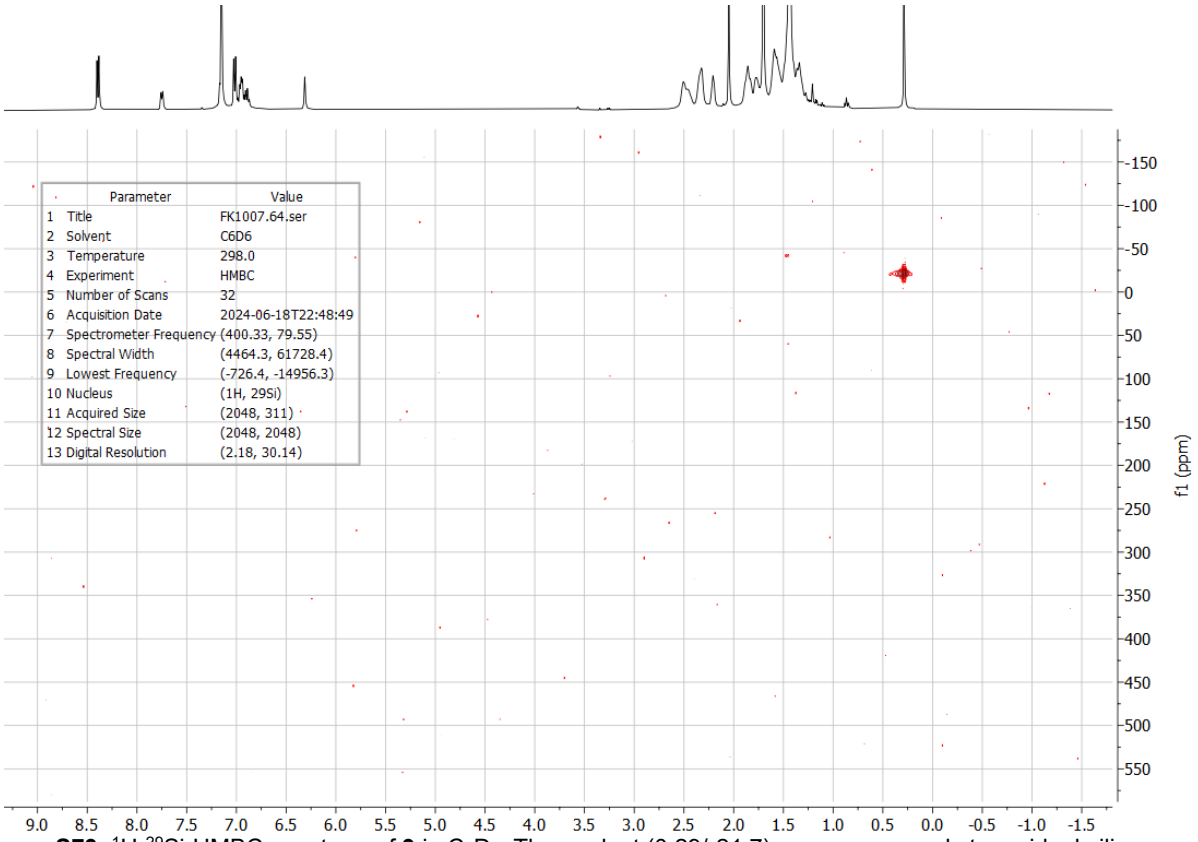


Figure S73. ^{1}H-^{29}Si-HMBC spectrum of **9** in C_6D_6. The peak at (0.29/-21.7) ppm corresponds to residual silicon grease that could not be removed due to similar solubility. The low intensity of the signal might result from the long relaxation time of **10**.

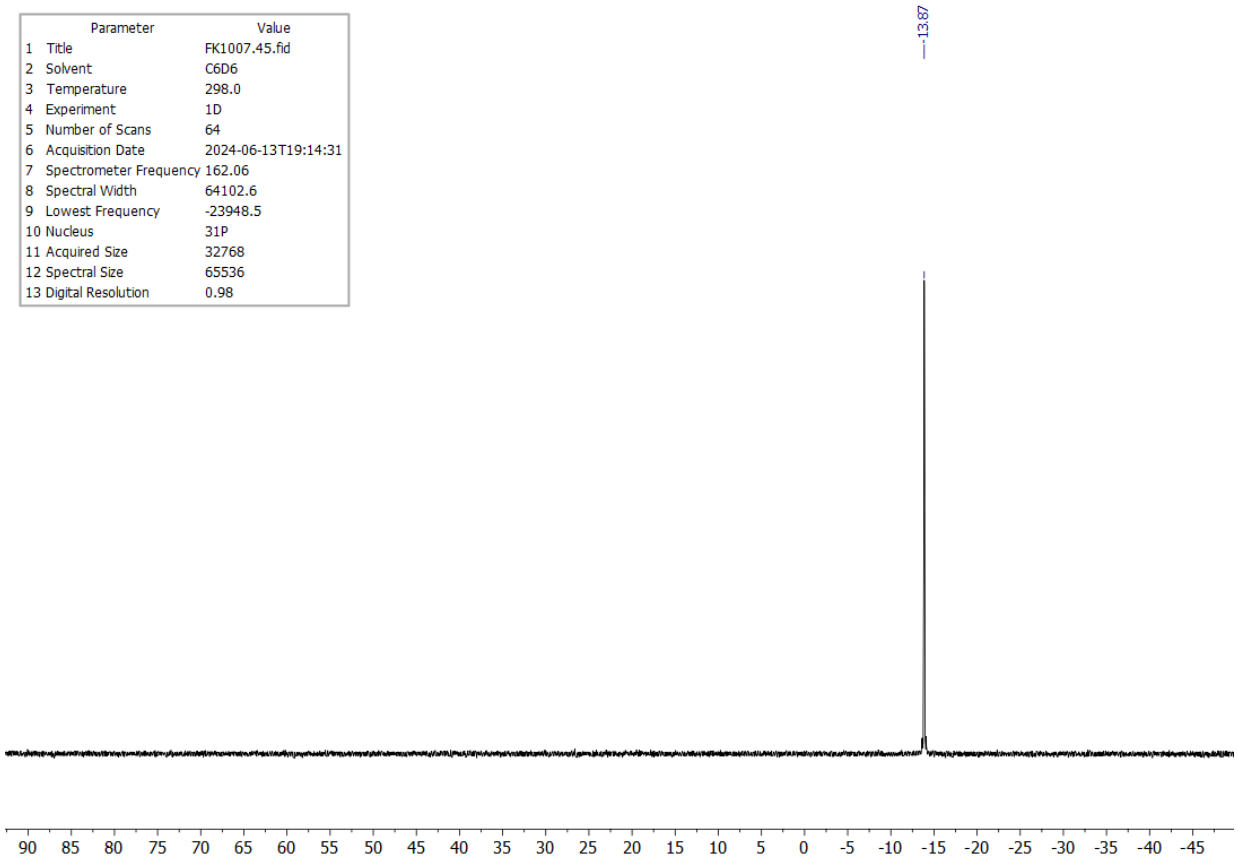


Figure S74. $^{31}P\{^{1}H\}$-NMR spectrum of **10** in C_6D_6.

6 Crystal Structure Analyses

6.1 Data collection and structure refinement details

Table S1 Data collection and structure refinement details for compounds **1**, **AYSi-2**, **AYSi-3** and **5_{Ts}**.

Compound	**2**	**AYSi-2**	**AYSi-3**	**5_{Ts}**
Formula	$C_{41}H_{45}N_2O_2P_1S_1Si_1$	$C_{41}H_{63}N_2O_2P_1S_1Si_1$	$C_{73}H_{79}N_6P_2Si_2$	$C_{42}H_{63}N_2O_2P_1S_3Si_1$
CCDC	2350309	2350308	2350310	2366468
Formula weight	688.91	707.05	1158.54	783.18
Temperature [K]	100(2)	100(2)	100(2)	100(2)
Wave length [Å]	1.54184	1.54184	1.54184	1.54184
Crystal system	monoclinic	triclinic	monoclinic	monoclinic
Space group	*P*21	*P*-1	*C*2/*c*	*P*21/*c*
a [Å]	9.86550(10)	9.87940(10)	64.6062(10)	13.63720(10)
b [Å]	10.66970(10)	9.96850(10)	10.33540(10)	14.83500(10)
c [Å]	17.54370(10)	21.1954(3)	19.79680(10)	20.8762(2)
α[°]	90	103.2980(10)	90	90
β [°]	94.8050(10)	98.3310(10)	94.6640(10)	100.6410(10)
γ [°]	90	90.0900(10)	90	90
Volumen [Å^3]	1840.19(3)	2008.66(4)	13175.16(17)	4150.79(6)
Z	2	2	8	4
Calc. density [Mg·m^{-3}]	1.243	1.169	1.168	1.253
μ (MoKα) [mm^{-1}]	1.792	1.643	1.297	2.557
F(000)	732	768	4936	1688
Crystal dimensions [mm]	0.210 x 0.120 x 0.070	0.220 x 0.130 x 0.060	0.404 x 0.135 x 0.100	0.149 x 0.112 x 0.052
Theta range θ [°]	2.527 to 67.984	4.335 to 67.996	2.745 to 78.241	3.297 to 67.073
Index ranges	-11 ≤ h ≤ 11	-9 ≤ h ≤ 11	-79 ≤ h ≤ 79	-16 ≤ h ≤ 16
	-12 ≤ k ≤ 12	-11 ≤ k ≤ 11	-12 ≤ k ≤ 13	-17 ≤ k ≤ 17
	-21 ≤ l ≤ 20	-25 ≤ l ≤ 22	-24 ≤ l ≤ 24	-24 ≤ l ≤ 24
Reflections collected	53970	24161	13797	54915
Independent reflections	6680 [*R*(int) = 0.0240]	7289 [*R*(int) = 0.0349]	13797 [R(int) = 0.434]	7406 [*R*(int) = 0.0604]
Data/Restraints/Parameter	6680/1/444	7289/0/443	13797/0/761	7406/0/467
Goodness-of-fit on F^2	1.014	1.055	1.153	1.051
Final R indices [I>2sigma(I)]	*R*1 = 0.0276, w*R*2 = 0.0731	*R*1 = 0.0358, w*R*2 = 0.0916	R1 = 0.0631, wR2 = 0.1857	*R*1 = 0.0387, w*R*2 = 0.1054
Largest diff. peak and hole [e·Å^{-3}]	0.426 and -0.259	0.496 and -0.355	0.966 and -0.463	0.501 and -0.477

Table S2 Data collection and structure refinement details for compounds **5**, **6**, and **7**.

Compound	**5_{CN}**	**6**	**7**	**8**
Formula	$C_{36}H_{38}N_3P_1S_2Si_1$	$C_{47}H_{69}N_2O_3P_1S_1Si_1$	$C_{94}H_{100}N_6O_2P_2Si_2$	$C_{36}H_{38}N_3O_3P_1Si_1$
CCDC	2366469	2350311	2350312	2429366
Formula weight	635.87	801.16	1463.91	619.75
Temperature [K]	100(2)	100(2)	100(2)	100(2)
Wave length [Å]	1.54184	1.54184	1.54184	1.54184
Crystal system	monoclinic	triclinic	monoclinic	monoclinic
Space group	*P*21/*c*	*P*-1	*I*2/*a*	$P2_1$/n
a [Å]	14.81430(10)	10.2796(2)	19.82520(10)	11.78680(10)
b [Å]	14.40780(10)	12.9114(2)	16.08220(10)	18.12460(10)
c [Å]	17.4032(2)	18.3044(2)	26.2606(2)	14.91140(10)
α[°]	90	74.2670(10)	90	90
β [°]	114.3500(10)	77.1070(10)	96.7770(10)	98.0340(10)
γ [°]	90	69.783(2)	90	90
Volumen [$Å^3$]	3384.13(6)	2171.70(7)	8314.24(9)	3154.27(4)
Z	4	2	4	4
Calc. density [$Mg·m^{-3}$]	1.248	1.225	1.170	1.305
μ (MoKα) [mm^{-1}]	2.431	1.598	1.148	1.464
F(000)	3120	868	3120	1312
Crystal dimensions [mm]	0.207 x 0.143 x 0.078	0.464 x 0.266 x 0.182	0.446 x 0.326 x 0.313	0.265 x 0.108 x 0.086
Theta range θ [°]	3.275 to 76.881	2.534 to 67.080	3.229 to 67.068	3.861 to 76.622
Index ranges	-18 ≤ h ≤ 18	-12 ≤ h ≤ 12	-23 ≤ h ≤ 22	-14 ≤ h ≤ 14
	-18 ≤ k ≤ 15	-15 ≤ k ≤ 15	-19 ≤ k ≤ 19	-15 ≤ k≤ 21
	-21 ≤ l ≤ 21	-19 ≤ l ≤ 21	-30 ≤ l ≤ 31	18 ≤ l≤ 18
Reflections collected	45900	71149	53814	23088
Independent reflections	7005 [R(int) = 0.0409]	7735 [*R*(int) = 0.0665]	7425 [R(int) = 0.0608]	6321 [R(int) = 0.0315]
Data/Restraints/Parameter	7005/0/394	7735/0/506	7425/0/515	6321/0/403
Goodness-of-fit on F^2	1.051	1.051	1.038	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0893	*R*1 = 0.0322, w*R*2 = 0.0821	R1 = 0.0405, wR2 = 0.1098	R1 = 0.0341, wR2 = 0.0895
Largest diff. peak and hole [$e·Å^{-3}$]	0.413 and -0.460	0.302 and -0.386	0.533 and -0.387	0.306 and -0.343

Table S3 Data collection and structure refinement details for compounds $\mathbf{8_{Ts}}$, $\mathbf{8_{CN}}$, and **9**.

Compound	$\mathbf{9_{Ts}}$	$\mathbf{9_{CN}}$	**10**
Formula	$C_{61}H_{81}N_4O_2P_1S_1Si_1$	$C_{48}H_{48}N_5P_1Si_1$	$C_{46}H_{72}N_3O_2P_1S_1Si$
CCDC	2366470	2366471	2366472
Formula weight	993.41	753.97	790.18
Temperature [K]	105(2)	109(2)	100(2)
Wave length [Å]	1.54184	1.54184	1.54184
Crystal system	triclinic	monoclinic	monoclinic
Space group	*P*-1	*P*21/*c*	*P*21/*n*
a [Å]	9.95910(10)	20.4704(2)	11.42850(10)
b [Å]	12.80600(10)	8.81830(10)	27.55120(10)
c [Å]	22.0685(2)	23.8065(2)	14.39760(10)
α[°]	76.2790(10)	90	90
β [°]	89.3570(10)	105.3050(10)	100.7750(10)
γ [°]	87.9160(10)	90	90
Volumen [Å^3]	2732.39(5)	4145.00(7)	4453.43(5)
Z	2	4	4
Calc. density [Mg·m^{-3}]	1.207	1.208	1.179
μ (MoKα) [mm^{-1}]	1.366	1.164	1.539
F(000)	1072	1600	1720
Crystal dimensions [mm]	0.060 x 0.050 x 0.040	0.310 x 0.160 x 0.080	0.170 x 0.130x 0.040
Theta range θ [°]	3.555 to 67.999	3.315 to 67.994	3.208 to 67.998
Index ranges	-11 ≤ h ≤ 11	-23 ≤ h ≤ 24	-13 ≤ h ≤ 13
	-14 ≤ k ≤ 15	-10 ≤ k ≤ 7	-30 ≤ k ≤ 33
	-26 ≤ l ≤ 26	-28 ≤ l ≤ 28	-17 ≤ l ≤ 17
Reflections collected	32168	31602	129827
Independent reflections	9892 [*R*(int) = 0.0319]	7555 [*R*(int) = 0.0402]	8107 [R(int) = 0.0687]
Data/Restraints/Parameter	9892/0/704	7555/0/502	8107/0/497
Goodness-of-fit on F^2	1.027	1.022	1.038
Final R indices [I>2sigma(I)]	*R*1 = 0.0345, w*R*2 = 0.0874	*R*1 = 0.0349, w*R*2 = 0.0879	R1 = 0.0330, wR2 = 0.0866
Largest diff. peak and hole [e·Å^{-3}]	0.403 and -0.364	0.348 and -0.306	0.297 and -0.396

6.2 Crystal structure determination of 2

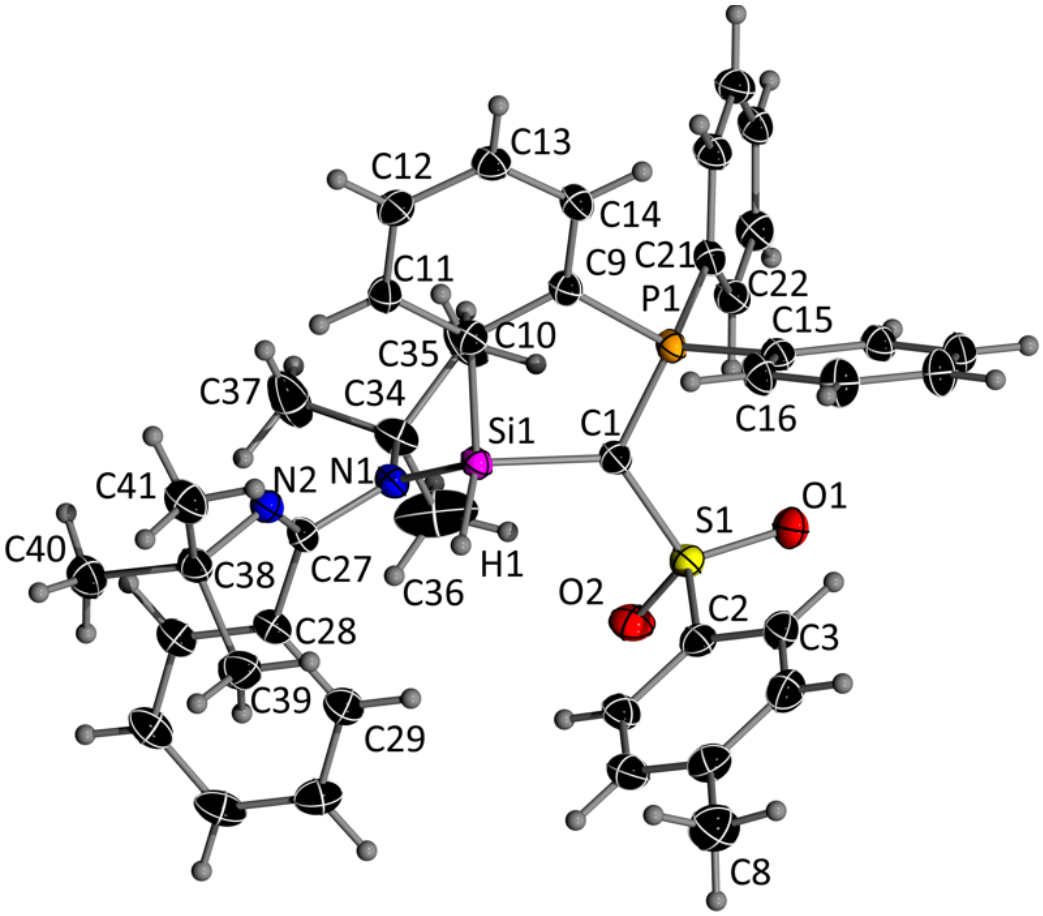


Figure S75. ORTEP of **2**. Thermal ellipsoids are drawn at 50% probability level.

Table S4. Atomic coordinates (x 10^4) and equivalentisotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

Atom	X	Y	Z	U(eq)
S1	0.29976(5)	0.71674(5)	0.67519(3)	0.02127(13)
P1	0.59015(5)	0.64291(5)	0.67962(3)	0.01850(13)
Si1	0.40822(6)	0.47376(6)	0.75812(3)	0.01873(14)
O1	0.35305(17)	0.83292(16)	0.64679(10)	0.0279(4)
N1	0.35636(19)	0.4750(2)	0.85117(11)	0.0215(4)
C1	0.4299(2)	0.6247(2)	0.70945(13)	0.0206(5)
O2	0.19962(17)	0.72343(18)	0.73103(10)	0.0291(4)
N2	0.3250(2)	0.26407(19)	0.83833(11)	0.0218(4)
C2	0.2146(2)	0.6411(2)	0.59442(14)	0.0234(5)
C3	0.2493(3)	0.6668(2)	0.52099(15)	0.0274(5)
C4	0.1841(3)	0.6033(3)	0.45886(15)	0.0315(6)
C5	0.0829(3)	0.5144(3)	0.46905(15)	0.0305(6)
C6	0.0497(2)	0.4909(3)	0.54285(15)	0.0293(5)
C7	0.1134(2)	0.5524(2)	0.60550(15)	0.0257(5)
C8	0.0132(3)	0.4446(3)	0.40244(17)	0.0420(7)
C9	0.6622(2)	0.4903(2)	0.70088(13)	0.0200(5)
C10	0.5827(2)	0.4115(2)	0.74327(13)	0.0206(5)
C11	0.6348(2)	0.2926(2)	0.76334(14)	0.0236(5)
C12	0.7591(2)	0.2536(2)	0.73929(15)	0.0265(5)
C13	0.8332(2)	0.3319(2)	0.69464(14)	0.0243(5)
C14	0.7855(2)	0.4510(2)	0.67587(14)	0.0225(5)
C15	0.6076(2)	0.6744(2)	0.57970(14)	0.0210(5)
C16	0.5952(3)	0.5759(2)	0.52738(15)	0.0265(5)
C17	0.6054(3)	0.5981(3)	0.45041(15)	0.0303(6)
C18	0.6270(3)	0.7195(3)	0.42530(14)	0.0296(5)
C19	0.6399(3)	0.8179(2)	0.47675(15)	0.0268(5)
C20	0.6306(2)	0.7965(2)	0.55435(14)	0.0229(5)
C21	0.6949(2)	0.7582(2)	0.73357(13)	0.0215(5)

C22	0.8368(2)	0.7481(2)	0.74251(15)	0.0248(5)
C23	0.9134(2)	0.8317(3)	0.78876(15)	0.0271(5)
C24	0.8495(3)	0.9267(2)	0.82596(15)	0.0255(5)
C25	0.7093(3)	0.9393(2)	0.81595(14)	0.0261(5)
C26	0.6320(2)	0.8549(2)	0.77018(15)	0.0247(5)
C27	0.2794(2)	0.3662(2)	0.86451(13)	0.0208(5)
C28	0.1448(2)	0.3872(2)	0.89702(14)	0.0223(5)
C29	0.0489(2)	0.4619(3)	0.85558(14)	0.0267(5)
C30	-0.0806(3)	0.4770(3)	0.87903(15)	0.0314(5)
C31	-0.1155(3)	0.4182(3)	0.94560(16)	0.0327(6)
C32	-0.0191(3)	0.3483(3)	0.98909(15)	0.0307(6)
C33	0.1104(2)	0.3325(2)	0.96489(14)	0.0258(5)
C34	0.3989(2)	0.5622(2)	0.91563(14)	0.0260(5)
C35	0.5310(3)	0.6256(3)	0.89958(15)	0.0352(6)
C36	0.2915(4)	0.6606(4)	0.9266(2)	0.0619(11)
C37	0.4283(4)	0.4858(4)	0.98912(16)	0.0503(9)
C38	0.2487(2)	0.1447(2)	0.82389(14)	0.0235(5)
C39	0.1214(3)	0.1666(3)	0.76962(17)	0.0329(6)
C40	0.2115(3)	0.0774(3)	0.89625(16)	0.0317(6)
C41	0.3457(3)	0.0597(3)	0.78505(17)	0.0320(6)

Table S5. Anisotropic displacement parameters(Å^2) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	0.0193(3)	0.0169(3)	0.0281(3)	-0.0006(2)	0.0045(2)	0.0023(2)
P1	0.0178(3)	0.0147(3)	0.0236(3)	0.0001(2)	0.0051(2)	0.0002(2)
Si1	0.0174(3)	0.0166(3)	0.0228(3)	-0.0001(2)	0.0052(2)	-0.0001(2)
O1	0.0291(9)	0.0173(8)	0.0372(10)	0.0021(7)	0.0024(7)	0.0009(7)
N1	0.0200(9)	0.0195(9)	0.0257(10)	-0.0004(8)	0.0055(7)	-0.0024(8)
C1	0.0195(11)	0.0171(11)	0.0255(11)	0.0002(9)	0.0050(9)	0.0011(9)
O2	0.0231(8)	0.0305(9)	0.0344(9)	-0.0042(8)	0.0075(7)	0.0047(7)
N2	0.0192(9)	0.0201(10)	0.0263(10)	0.0013(8)	0.0035(8)	-0.0002(8)
C2	0.0195(10)	0.0208(11)	0.0300(12)	0.0006(10)	0.0028(9)	0.0044(9)
C3	0.0264(12)	0.0239(13)	0.0322(13)	0.0058(10)	0.0036(10)	0.0026(10)
C4	0.0341(14)	0.0337(14)	0.0270(13)	0.0050(11)	0.0032(10)	0.0053(11)
C5	0.0281(13)	0.0301(14)	0.0328(13)	-	-	0.0050(10)
C6	0.0212(11)	0.0307(13)	0.0361(13)	-	0.0041(10)	-
C7	0.0214(11)	0.0278(13)	0.0288(12)	0.0003(10)	0.0066(9)	0.0002(10)
C8	0.0425(16)	0.0477(18)	0.0349(15)	-	-	-
C9	0.0203(10)	0.0162(11)	0.0236(11)	-0.0020(9)	0.0026(8)	-0.0003(9)
C10	0.0205(11)	0.0186(12)	0.0229(12)	-0.0025(9)	0.0034(9)	0.0012(9)
C11	0.0232(12)	0.0203(12)	0.0277(12)	0.0039(10)	0.0041(9)	0.0005(9)
C12	0.0232(12)	0.0211(12)	0.0353(14)	0.0018(10)	0.0035(10)	0.0046(9)
C13	0.0204(11)	0.0225(12)	0.0305(12)	-	0.0050(9)	0.0028(10)
C14	0.0220(11)	0.0204(12)	0.0259(12)	-0.0004(9)	0.0069(9)	-0.0016(9)
C15	0.0180(10)	0.0186(11)	0.0269(12)	0.0005(9)	0.0047(9)	0.0016(8)
C16	0.0301(13)	0.0178(12)	0.0323(13)	0.0000(10)	0.0066(10)	-
C17	0.0406(15)	0.0232(13)	0.0274(13)	-	0.0050(11)	-
C18	0.0371(13)	0.0298(13)	0.0227(12)	0.0032(11)	0.0068(10)	-
C19	0.0280(13)	0.0219(12)	0.0310(13)	0.0043(10)	0.0048(10)	-
C20	0.0220(12)	0.0186(12)	0.0285(13)	-0.0005(9)	0.0039(9)	-0.0010(9)
C21	0.0230(12)	0.0191(12)	0.0227(12)	0.0022(9)	0.0042(9)	-0.0022(9)
C22	0.0222(12)	0.0229(13)	0.0298(13)	-	0.0064(9)	0.0011(10)
C23	0.0201(11)	0.0283(13)	0.0331(13)	0.0001(11)	0.0039(10)	-
C24	0.0266(12)	0.0212(12)	0.0283(12)	0.0016(10)	0.0009(10)	-
C25	0.0278(12)	0.0200(12)	0.0310(13)	-	0.0063(10)	0.0016(9)
C26	0.0210(11)	0.0211(12)	0.0324(13)	0.0007(10)	0.0046(9)	-0.0005(9)
C27	0.0210(11)	0.0219(12)	0.0200(11)	0.0023(9)	0.0043(9)	-0.0012(9)
C28	0.0197(11)	0.0224(12)	0.0250(12)	-0.0031(9)	0.0042(9)	-0.0030(9)
C29	0.0248(12)	0.0286(13)	0.0270(12)	-	0.0043(9)	-
C30	0.0236(12)	0.0377(14)	0.0326(13)	-	0.0017(10)	0.0055(11)

C31	0.0218(12)	0.0433(16)	0.0342(14)	-	0.0085(10)	-
C32	0.0288(13)	0.0370(14)	0.0278(13)	-	0.0113(10)	-
C33	0.0238(12)	0.0270(13)	0.0272(12)	-	0.0056(9)	-
C34	0.0240(12)	0.0289(13)	0.0255(12)	-	0.0045(10)	-
C35	0.0387(15)	0.0398(16)	0.0278(13)	-	0.0063(11)	-
C36	0.0426(18)	0.063(2)	0.078(3)	-0.050(2)	-	0.0167(17)
C37	0.060(2)	0.062(2)	0.0276(14)	0.0058(15)	-	-
C38	0.0217(11)	0.0198(11)	0.0295(12)	0.0005(10)	0.0043(9)	-
C39	0.0284(13)	0.0276(14)	0.0418(15)	-	-	-
C40	0.0330(14)	0.0256(13)	0.0371(15)	0.0015(11)	0.0065(11)	-
C41	0.0311(13)	0.0248(13)	0.0410(15)	-	0.0087(11)	-

6.3 Crystal structure determination of AYSi-2

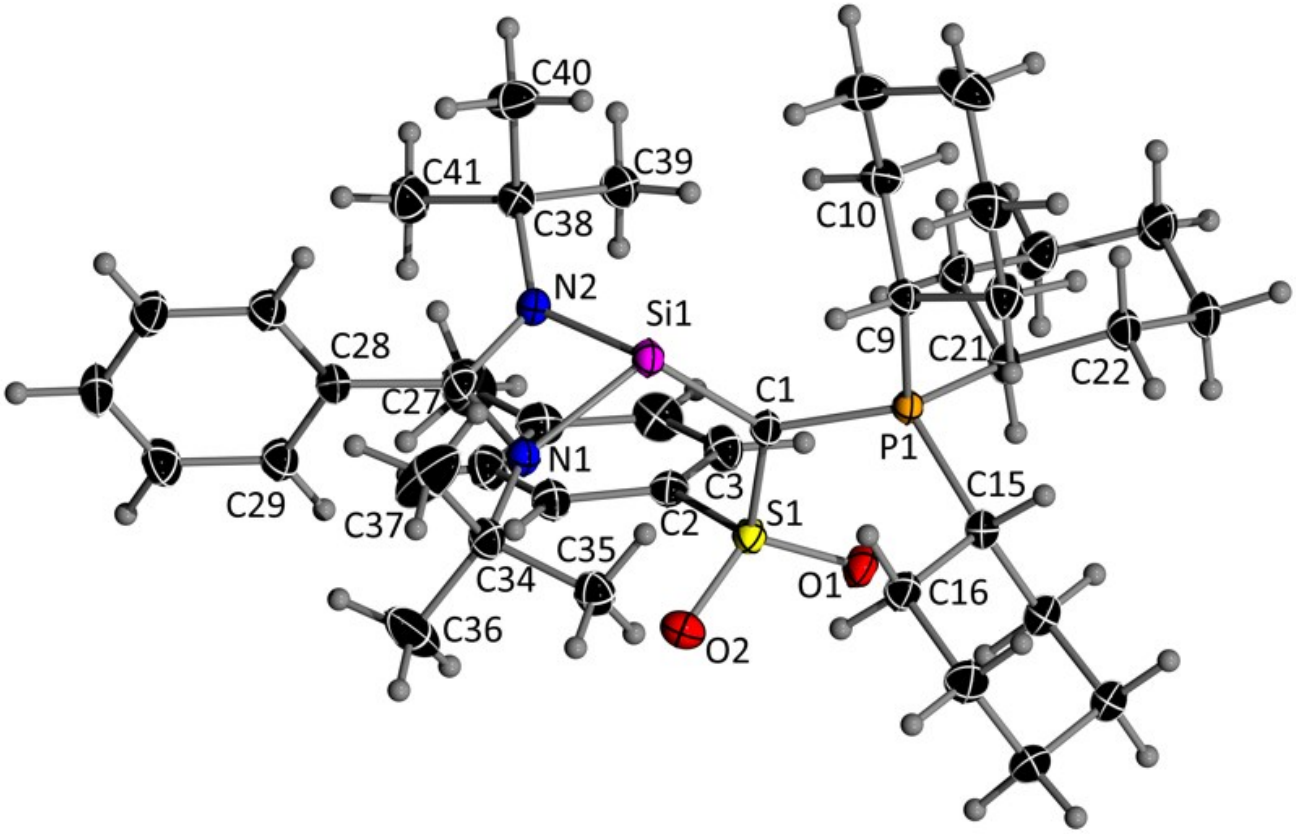


Figure S76. ORTEP of **AYSi-2**. Thermal ellipsoids are drawn at 50% probability level.

Table S6. Atomic coordinates (x 10^4) and equivalentisotropic displacement parameters ($Å^2$x 10^3) for **AYSi-2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

Atom	X	Y	Z	U(eq)
S1	0.31498(3)	0.55339(4)	0.28710(2)	0.01786(10)
P1	0.30444(3)	0.65677(4)	0.17018(2)	0.01592(9)
Si1	0.59010(4)	0.55588(4)	0.22429(2)	0.01825(10)
O1	0.17759(10)	0.60635(12)	0.27829(5)	0.0243(2)
N1	0.63354(12)	0.40748(13)	0.26301(6)	0.0198(3)
O2	0.32215(11)	0.40747(11)	0.28643(5)	0.0236(2)
N2	0.70082(12)	0.61638(13)	0.30717(6)	0.0194(3)
C1	0.40612(14)	0.59790(15)	0.23212(7)	0.0171(3)
C2	0.38619(15)	0.63759(15)	0.36880(7)	0.0195(3)
C3	0.33637(16)	0.76196(17)	0.39999(8)	0.0253(3)
C4	0.38982(18)	0.82190(17)	0.46464(8)	0.0291(4)

C5	0.49293(17)	0.76019(17)	0.49905(8)	0.0279(3)
C6	0.53917(16)	0.63437(17)	0.46745(8)	0.0266(3)
C7	0.48644(15)	0.57283(16)	0.40311(7)	0.0225(3)
C8	0.5546(2)	0.8265(2)	0.56882(9)	0.0400(4)
C9	0.42101(15)	0.68185(15)	0.11225(7)	0.0187(3)
C10	0.51330(16)	0.81259(16)	0.13924(8)	0.0235(3)
C11	0.62119(17)	0.82026(17)	0.09513(9)	0.0307(4)
C12	0.5527(2)	0.81978(18)	0.02596(9)	0.0351(4)
C13	0.46268(18)	0.69032(19)	-0.00187(8)	0.0317(4)
C14	0.35494(16)	0.67435(18)	0.04138(8)	0.0269(3)
C15	0.16774(14)	0.53519(15)	0.11819(7)	0.0194(3)
C16	0.22103(15)	0.38862(15)	0.10269(8)	0.0225(3)
C17	0.11841(17)	0.29014(17)	0.05176(8)	0.0282(3)
C18	-0.02277(16)	0.29294(17)	0.07313(9)	0.0285(4)
C19	-0.07384(15)	0.43944(17)	0.08861(8)	0.0256(3)
C20	0.02754(15)	0.53414(16)	0.14161(8)	0.0235(3)
C21	0.21252(14)	0.81521(15)	0.19757(7)	0.0193(3)
C22	0.13978(15)	0.87405(16)	0.14102(8)	0.0229(3)
C23	0.04609(16)	0.98877(16)	0.16771(8)	0.0270(3)
C24	0.12787(16)	1.10278(17)	0.21959(9)	0.0295(4)
C25	0.20447(16)	1.04665(17)	0.27546(8)	0.0271(3)
C26	0.29673(15)	0.92915(15)	0.24978(7)	0.0216(3)
C27	0.72617(14)	0.48570(15)	0.30986(7)	0.0190(3)
C28	0.83824(15)	0.43403(15)	0.35225(7)	0.0208(3)
C29	0.81028(16)	0.38763(16)	0.40642(8)	0.0244(3)
C30	0.91372(17)	0.33628(18)	0.44488(8)	0.0297(4)
C31	1.04559(17)	0.33010(18)	0.42922(8)	0.0301(4)
C32	1.07449(16)	0.37728(17)	0.37600(8)	0.0271(3)
C33	0.97143(15)	0.42939(16)	0.33754(8)	0.0234(3)
C34	0.63456(16)	0.25856(16)	0.23224(8)	0.0245(3)
C35	0.50998(16)	0.22845(16)	0.17914(8)	0.0261(3)
C36	0.6213(3)	0.1705(2)	0.28050(11)	0.0543(6)
C37	0.76280(19)	0.2266(2)	0.19933(13)	0.0545(6)
C38	0.77461(15)	0.74846(15)	0.34102(8)	0.0220(3)
C39	0.66555(16)	0.85720(16)	0.34882(8)	0.0260(3)
C40	0.85038(19)	0.74694(18)	0.40897(9)	0.0336(4)
C41	0.87477(17)	0.78386(18)	0.29810(9)	0.0318(4)

Table S7. Anisotropic displacement parameters(Å^2) for **AYSi-2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	0.01478(17)	0.02166(19)	0.01836(18)	0.00673(13)	0.00311(13)	0.00166(13)
P1	0.01366(17)	0.01720(18)	0.01745(18)	0.00553(14)	0.00168(13)	0.00285(13)
Si1	0.01534(19)	0.0212(2)	0.0199(2)	0.00786(15)	0.00324(15)	0.00416(15)
O1	0.0137(5)	0.0354(6)	0.0265(6)	0.0120(5)	0.0038(4)	0.0035(4)
N1	0.0173(6)	0.0203(6)	0.0226(6)	0.0070(5)	0.0029(5)	0.0036(5)
O2	0.0270(6)	0.0213(5)	0.0243(5)	0.0071(4)	0.0062(4)	-0.0006(4)
N2	0.0161(6)	0.0205(6)	0.0224(6)	0.0077(5)	0.0012(5)	0.0013(5)
C1	0.0146(6)	0.0197(7)	0.0181(7)	0.0065(6)	0.0024(5)	0.0033(5)
C2	0.0177(7)	0.0242(7)	0.0188(7)	0.0073(6)	0.0062(6)	0.0008(6)
C3	0.0249(8)	0.0277(8)	0.0256(8)	0.0083(6)	0.0079(6)	0.0074(6)
C4	0.0351(9)	0.0274(8)	0.0254(8)	0.0026(7)	0.0118(7)	0.0056(7)
C5	0.0328(9)	0.0306(9)	0.0210(8)	0.0061(6)	0.0059(7)	-0.0019(7)
C6	0.0270(8)	0.0321(9)	0.0223(8)	0.0109(7)	0.0014(6)	0.0023(7)
C7	0.0224(7)	0.0252(8)	0.0220(7)	0.0080(6)	0.0055(6)	0.0036(6)
C8	0.0538(12)	0.0402(10)	0.0232(9)	0.0032(8)	0.0036(8)	-0.0011(9)
C9	0.0179(7)	0.0197(7)	0.0196(7)	0.0061(6)	0.0038(6)	0.0024(6)
C10	0.0239(8)	0.0205(8)	0.0267(8)	0.0051(6)	0.0066(6)	0.0001(6)
C11	0.0292(8)	0.0245(8)	0.0392(9)	0.0031(7)	0.0146(7)	-0.0034(7)
C12	0.0442(10)	0.0302(9)	0.0394(10)	0.0150(8)	0.0235(8)	0.0056(8)
C13	0.0353(9)	0.0395(10)	0.0244(8)	0.0130(7)	0.0089(7)	0.0034(7)
C14	0.0262(8)	0.0356(9)	0.0210(8)	0.0114(7)	0.0030(6)	0.0047(7)
C15	0.0181(7)	0.0206(7)	0.0197(7)	0.0062(6)	0.0008(6)	0.0019(6)
C16	0.0183(7)	0.0213(8)	0.0267(8)	0.0046(6)	0.0015(6)	0.0017(6)
C17	0.0277(8)	0.0223(8)	0.0317(9)	0.0028(7)	0.0004(7)	-0.0005(6)

C18	0.0231(8)	0.0256(8)	0.0352(9)	0.0087(7)	-0.0036(7)	-0.0046(6)
C19	0.0187(7)	0.0285(8)	0.0295(8)	0.0102(7)	-0.0020(6)	-0.0015(6)
C20	0.0171(7)	0.0266(8)	0.0266(8)	0.0070(6)	0.0015(6)	0.0014(6)
C21	0.0155(7)	0.0200(7)	0.0229(7)	0.0059(6)	0.0027(6)	0.0044(5)
C22	0.0202(7)	0.0217(8)	0.0265(8)	0.0071(6)	0.0001(6)	0.0047(6)
C23	0.0202(7)	0.0237(8)	0.0371(9)	0.0097(7)	0.0002(7)	0.0074(6)
C24	0.0230(8)	0.0211(8)	0.0421(10)	0.0040(7)	0.0027(7)	0.0073(6)
C25	0.0210(7)	0.0256(8)	0.0310(8)	-0.0011(7)	0.0040(6)	0.0053(6)
C26	0.0178(7)	0.0211(7)	0.0246(8)	0.0033(6)	0.0017(6)	0.0043(6)
C27	0.0153(7)	0.0227(7)	0.0216(7)	0.0083(6)	0.0061(6)	0.0038(5)
C28	0.0187(7)	0.0203(7)	0.0239(8)	0.0071(6)	0.0015(6)	0.0027(6)
C29	0.0205(7)	0.0279(8)	0.0277(8)	0.0112(7)	0.0054(6)	0.0046(6)
C30	0.0309(9)	0.0365(9)	0.0255(8)	0.0157(7)	0.0031(7)	0.0050(7)
C31	0.0254(8)	0.0364(9)	0.0299(9)	0.0141(7)	-0.0012(7)	0.0097(7)
C32	0.0189(7)	0.0323(9)	0.0311(9)	0.0096(7)	0.0030(6)	0.0049(6)
C33	0.0209(7)	0.0262(8)	0.0250(8)	0.0093(6)	0.0046(6)	0.0030(6)
C34	0.0215(7)	0.0187(7)	0.0321(8)	0.0052(6)	0.0011(6)	0.0041(6)
C35	0.0286(8)	0.0220(8)	0.0261(8)	0.0040(6)	0.0019(6)	0.0036(6)
C36	0.0847(16)	0.0285(10)	0.0433(12)	0.0181(9)	-0.0275(11)	-0.0197(10)
C37	0.0246(9)	0.0383(11)	0.0844(17)	-0.0213(11)	0.0125(10)	0.0056(8)
C38	0.0193(7)	0.0207(7)	0.0257(8)	0.0066(6)	0.0002(6)	-0.0001(6)
C39	0.0239(8)	0.0227(8)	0.0316(8)	0.0067(6)	0.0040(6)	0.0032(6)
C40	0.0367(9)	0.0271(9)	0.0322(9)	0.0073(7)	-0.0110(7)	-0.0026(7)
C41	0.0254(8)	0.0279(8)	0.0429(10)	0.0062(7)	0.0113(7)	-0.0031(7)

6.4 Crystal structure determination of AYSi-3

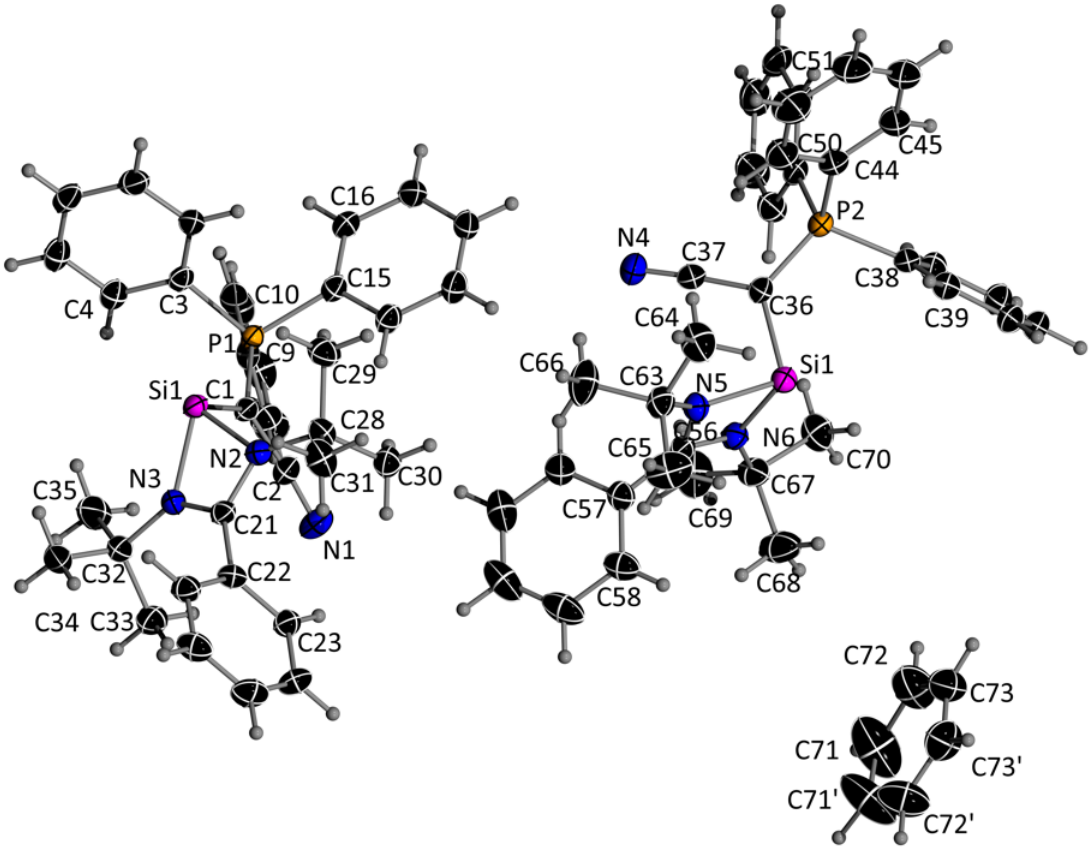


Figure S77. ORTEP of **AYSi-3**. Ellipsoids are drawn at the 50% probability level.

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **AYSi-3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

atom	x	y	z	U(eq)
P1	0.67894(2)	0.20481(6)	0.71480(3)	0.02354(15)
P2	0.55885(2)	0.97076(7)	0.68663(3)	0.02762(16)
Si1	0.71035(2)	0.25260(7)	0.60514(3)	0.02553(16)
Si2	0.56513(2)	0.85289(7)	0.54184(4)	0.02792(17)
N1	0.65733(4)	0.1522(3)	0.53243(12)	0.0381(6)
N2	0.70189(3)	0.3533(2)	0.52812(11)	0.0259(4)
N3	0.71062(3)	0.1548(2)	0.52533(11)	0.0276(5)
N4	0.59624(4)	0.6992(3)	0.69411(14)	0.0404(6)
N5	0.56293(3)	0.6722(2)	0.53249(11)	0.0285(5)
N6	0.59029(3)	0.7802(2)	0.51768(11)	0.0283(5)
C5	0.73421(4)	0.0953(3)	0.80923(14)	0.0335(6)
C6	0.74267(4)	0.2111(3)	0.83364(14)	0.0357(6)
C7	0.73168(4)	0.3254(3)	0.82420(14)	0.0348(6)
C8	0.71184(4)	0.3247(3)	0.79061(13)	0.0305(6)
C9	0.66376(4)	0.0711(3)	0.74447(14)	0.0279(5)
C10	0.66345(4)	0.0493(3)	0.81443(14)	0.0326(6)
C11	0.64983(5)	-0.0396(3)	0.83864(16)	0.0373(6)
C1	0.68420(4)	0.2006(3)	0.63196(12)	0.0254(5)
C2	0.66866(4)	0.1741(3)	0.57955(13)	0.0291(5)
C12	0.63642(5)	-0.1077(3)	0.79338(18)	0.0415(7)
C13	0.63722(5)	-0.0906(3)	0.72450(18)	0.0417(7)
C14	0.65081(5)	-0.0008(3)	0.69934(15)	0.0351(6)
C15	0.66374(4)	0.3441(3)	0.73805(13)	0.0263(5)
C16	0.65928(4)	0.3700(3)	0.80457(14)	0.0332(6)
C17	0.64591(4)	0.4706(3)	0.81807(14)	0.0351(6)
C18	0.63710(4)	0.5462(3)	0.76548(15)	0.0339(6)
C19	0.64163(4)	0.5225(3)	0.69999(15)	0.0357(6)
C20	0.65496(4)	0.4218(3)	0.68578(13)	0.0303(5)
C21	0.70591(4)	0.2577(3)	0.48584(13)	0.0251(5)
C22	0.70679(4)	0.2660(3)	0.41092(13)	0.0262(5)
C23	0.68874(4)	0.2679(3)	0.36766(13)	0.0297(5)
C24	0.68988(5)	0.2785(3)	0.29827(14)	0.0362(6)
C25	0.70902(5)	0.2880(3)	0.27155(14)	0.0400(7)
C26	0.72703(5)	0.2854(3)	0.31425(15)	0.0370(6)
C27	0.72601(4)	0.2746(3)	0.38361(14)	0.0311(6)
C28	0.69460(4)	0.4871(3)	0.51554(14)	0.0300(5)
C29	0.69902(5)	0.5584(3)	0.58309(16)	0.0382(6)
C30	0.67109(4)	0.4858(3)	0.49618(15)	0.0349(6)
C31	0.70540(5)	0.5561(3)	0.45996(17)	0.0413(7)
C32	0.71553(5)	0.0199(3)	0.50945(14)	0.0334(6)
C33	0.70027(5)	-0.0316(3)	0.45255(16)	0.0379(6)
C34	0.73780(5)	0.0067(3)	0.48935(19)	0.0462(8)
C35	0.71333(7)	-0.0578(3)	0.57408(17)	0.0502(9)
C36	0.57090(4)	0.8654(3)	0.63652(14)	0.0281(5)
C37	0.58481(4)	0.7763(3)	0.66962(14)	0.0313(6)

C38	0.57105(4)	1.1264(3)	0.70400(15)	0.0351(6)
C39	0.59214(5)	1.1409(3)	0.69641(18)	0.0441(7)
C40	0.60178(6)	1.2597(4)	0.7105(2)	0.0546(9)
C41	0.59037(6)	1.3640(4)	0.7304(2)	0.0540(9)
C42	0.56940(6)	1.3493(3)	0.73867(19)	0.0499(8)
C43	0.55978(5)	1.2312(3)	0.72572(18)	0.0431(7)
C44	0.55589(4)	0.8976(3)	0.76861(14)	0.0349(6)
C45	0.56002(5)	0.9635(4)	0.82957(15)	0.0437(8)
C46	0.55774(5)	0.9007(5)	0.89152(16)	0.0546(10)
C47	0.55123(7)	0.7735(4)	0.89191(18)	0.0570(10)
C48	0.54709(7)	0.7065(4)	0.83170(17)	0.0559(10)
C49	0.54975(5)	0.7681(3)	0.77047(15)	0.0416(7)
C50	0.53324(4)	1.0113(3)	0.64826(13)	0.0278(5)
C51	0.51561(4)	0.9497(3)	0.66902(14)	0.0317(6)
C52	0.49616(4)	0.9757(3)	0.63610(16)	0.0362(6)
C53	0.49429(4)	1.0618(3)	0.58233(15)	0.0364(6)
C54	0.51178(5)	1.1234(3)	0.56169(14)	0.0348(6)
C55	0.53122(4)	1.0991(3)	0.59466(13)	0.0304(5)
C56	0.58205(4)	0.6629(3)	0.51086(12)	0.0261(5)
C57	0.59204(4)	0.5436(3)	0.48607(14)	0.0300(5)
C58	0.59057(5)	0.5084(3)	0.41821(15)	0.0372(6)
C59	0.60001(5)	0.3949(4)	0.39785(18)	0.0486(8)
C60	0.61124(6)	0.3184(3)	0.4454(2)	0.0524(9)
C61	0.61278(5)	0.3533(3)	0.5129(2)	0.0495(8)
C62	0.60312(5)	0.4640(3)	0.53345(17)	0.0397(7)
C63	0.54556(4)	0.5810(3)	0.52865(15)	0.0351(6)
C64	0.52815(5)	0.6476(3)	0.56340(18)	0.0428(7)
C65	0.53733(6)	0.5663(4)	0.45274(19)	0.0566(10)
C66	0.55120(6)	0.4535(4)	0.5600(2)	0.0583(10)
C67	0.61015(4)	0.8322(3)	0.49670(15)	0.0331(6)
C68	0.61027(6)	0.8304(4)	0.42028(18)	0.0543(9)
C69	0.62855(5)	0.7573(4)	0.5302(2)	0.0533(9)
C70	0.61113(5)	0.9712(3)	0.5229(2)	0.0500(8)
C71	0.49714(9)	0.4605(5)	0.2812(3)	0.0929(19)
C72	0.49521(8)	0.5764(5)	0.3158(2)	0.0685(12)
C73	0.49789(6)	0.6924(4)	0.28246(19)	0.0542(9)
C3	0.70329(4)	0.2084(3)	0.76623(12)	0.0249(5)
C4	0.71456(4)	0.0932(3)	0.77551(13)	0.0292(5)

Table S9. Anisotropic displacement parameters(Å^2) for **AYSi-3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P1	0.0208(3)	0.0289(3)	0.0204(3)	0.0021(2)	-0.0013(2)	0.0017(2)
P2	0.0242(3)	0.0310(3)	0.0266(3)	-0.0050(3)	-0.0044(2)	0.0039(2)
Si1	0.0221(3)	0.0344(4)	0.0198(3)	-0.0024(3)	-0.0007(2)	0.0019(3)
Si2	0.0255(3)	0.0319(4)	0.0260(3)	-0.0002(3)	-0.0001(3)	0.0030(3)
N1	0.0309(12)	0.0524(16)	0.0299(12)	0.0035(11)	-0.0052(10)	-0.0054(11)
N2	0.0267(10)	0.0280(11)	0.0228(10)	-0.0018(8)	0.0014(8)	-0.0016(8)
N3	0.0304(11)	0.0282(11)	0.0237(10)	-0.0022(8)	-0.0002(8)	0.0081(9)

N4	0.0338(13)	0.0411(14)	0.0445(14)	-0.0040(11)	-0.0088(11)	0.0101(11)
N5	0.0233(10)	0.0336(12)	0.0284(11)	-0.0031(9)	0.0016(8)	-0.0016(9)
N6	0.0234(10)	0.0315(11)	0.0303(11)	-0.0006(9)	0.0037(8)	0.0005(9)
C5	0.0266(13)	0.0467(16)	0.0278(13)	0.0115(12)	0.0050(10)	0.0065(12)
C6	0.0215(12)	0.0619(19)	0.0234(12)	0.0008(12)	0.0010(10)	0.0041(12)
C7	0.0262(13)	0.0499(17)	0.0280(13)	-0.0101(12)	0.0007(10)	-0.0023(12)
C8	0.0269(13)	0.0386(15)	0.0257(12)	-0.0061(11)	-0.0002(10)	0.0060(11)
C9	0.0225(12)	0.0282(13)	0.0329(13)	0.0049(10)	0.0019(10)	0.0058(10)
C10	0.0302(13)	0.0358(14)	0.0323(14)	0.0040(11)	0.0048(11)	0.0057(11)
C11	0.0395(15)	0.0372(15)	0.0370(15)	0.0085(12)	0.0141(12)	0.0082(12)
C1	0.0226(11)	0.0313(13)	0.0217(11)	0.0004(10)	-0.0025(9)	0.0002(10)
C2	0.0244(12)	0.0362(14)	0.0263(12)	0.0040(11)	-0.0007(10)	-0.0005(10)
C12	0.0385(16)	0.0334(15)	0.0546(19)	0.0053(14)	0.0165(14)	-0.0007(12)
C13	0.0374(15)	0.0371(16)	0.0508(18)	-0.0017(14)	0.0036(13)	-0.0073(13)
C14	0.0362(15)	0.0349(15)	0.0340(14)	0.0017(12)	0.0011(11)	-0.0012(12)
C15	0.0209(11)	0.0318(13)	0.0257(12)	0.0021(10)	-0.0006(9)	-0.0002(10)
C16	0.0329(14)	0.0396(15)	0.0259(13)	-0.0003(11)	-0.0042(10)	0.0071(12)
C17	0.0303(13)	0.0448(16)	0.0298(13)	-0.0070(12)	0.0001(11)	0.0055(12)
C18	0.0254(13)	0.0341(14)	0.0412(15)	-0.0066(12)	-0.0032(11)	0.0054(11)
C19	0.0329(14)	0.0362(15)	0.0370(15)	0.0059(12)	-0.0028(11)	0.0073(12)
C20	0.0287(13)	0.0364(14)	0.0256(12)	0.0048(11)	-0.0001(10)	0.0030(11)
C21	0.0206(11)	0.0317(13)	0.0226(12)	-0.0029(10)	-0.0002(9)	-0.0006(9)
C22	0.0302(13)	0.0270(12)	0.0215(12)	-0.0030(9)	0.0031(10)	-0.0012(10)
C23	0.0263(12)	0.0367(14)	0.0259(12)	-0.0014(11)	0.0018(10)	0.0007(11)
C24	0.0404(15)	0.0438(16)	0.0235(13)	0.0002(11)	-0.0037(11)	-0.0029(13)
C25	0.0528(18)	0.0455(17)	0.0226(13)	0.0013(12)	0.0079(12)	-0.0015(14)
C26	0.0381(15)	0.0414(16)	0.0334(14)	-0.0048(12)	0.0143(12)	-0.0057(12)
C27	0.0282(13)	0.0347(14)	0.0306(13)	-0.0052(11)	0.0030(10)	-0.0027(11)
C28	0.0315(13)	0.0287(13)	0.0304(13)	-0.0009(11)	0.0062(10)	0.0020(10)
C29	0.0430(16)	0.0313(14)	0.0402(16)	-0.0089(12)	0.0027(13)	-0.0028(12)
C30	0.0338(14)	0.0384(15)	0.0323(14)	0.0031(12)	0.0009(11)	0.0079(12)
C31	0.0436(17)	0.0337(15)	0.0487(18)	0.0061(13)	0.0155(14)	0.0028(13)
C32	0.0392(15)	0.0291(14)	0.0305(13)	-0.0056(11)	-0.0059(11)	0.0080(11)
C33	0.0435(16)	0.0291(14)	0.0395(15)	-0.0026(12)	-0.0065(13)	-0.0004(12)
C34	0.0356(16)	0.0453(18)	0.0557(19)	-0.0216(15)	-0.0078(14)	0.0112(13)
C35	0.077(2)	0.0347(16)	0.0378(16)	0.0028(13)	-0.0012(16)	0.0156(16)
C36	0.0210(11)	0.0313(13)	0.0311(13)	-0.0042(10)	-0.0028(10)	0.0026(10)
C37	0.0294(13)	0.0333(14)	0.0304(13)	-0.0067(11)	-0.0033(11)	0.0011(11)
C38	0.0315(14)	0.0358(15)	0.0365(15)	-0.0083(12)	-0.0067(11)	-0.0004(11)
C39	0.0331(15)	0.0439(18)	0.0544(19)	-0.0126(15)	-0.0011(13)	-0.0043(13)
C40	0.0400(18)	0.054(2)	0.069(2)	-0.0144(18)	0.0003(16)	-0.0146(16)
C41	0.058(2)	0.0429(19)	0.058(2)	-0.0134(16)	-0.0102(17)	-0.0102(16)
C42	0.054(2)	0.0405(18)	0.052(2)	-0.0148(15)	-0.0123(16)	0.0037(15)
C43	0.0360(16)	0.0408(17)	0.0508(18)	-0.0150(14)	-0.0065(13)	0.0028(13)
C44	0.0306(13)	0.0477(17)	0.0251(13)	-0.0032(12)	-0.0056(10)	0.0129(12)
C45	0.0324(15)	0.064(2)	0.0329(15)	-0.0107(14)	-0.0075(12)	0.0109(14)
C46	0.0445(18)	0.093(3)	0.0250(14)	-0.0070(17)	-0.0055(13)	0.0276(19)
C47	0.073(3)	0.065(2)	0.0333(17)	0.0112(16)	0.0038(16)	0.033(2)
C48	0.081(3)	0.053(2)	0.0346(17)	0.0099(15)	0.0078(17)	0.0255(19)

C49	0.058(2)	0.0394(16)	0.0268(14)	0.0034(12)	0.0016(13)	0.0180(14)
C50	0.0266(12)	0.0296(13)	0.0262(12)	-0.0065(10)	-0.0034(10)	0.0035(10)
C51	0.0299(13)	0.0334(14)	0.0316(13)	0.0019(11)	0.0008(11)	0.0036(11)
C52	0.0273(13)	0.0394(16)	0.0413(16)	-0.0038(12)	-0.0011(11)	0.0010(11)
C53	0.0298(14)	0.0422(16)	0.0356(14)	-0.0065(12)	-0.0068(11)	0.0082(12)
C54	0.0387(15)	0.0370(15)	0.0279(13)	0.0004(11)	-0.0029(11)	0.0099(12)
C55	0.0305(13)	0.0316(13)	0.0287(13)	-0.0019(11)	0.0013(10)	0.0025(11)
C56	0.0225(12)	0.0336(13)	0.0219(11)	-0.0009(10)	-0.0001(9)	0.0015(10)
C57	0.0254(12)	0.0327(14)	0.0323(13)	-0.0022(11)	0.0051(10)	-0.0012(10)
C58	0.0365(15)	0.0417(16)	0.0349(14)	-0.0064(12)	0.0120(12)	-0.0079(12)
C59	0.0500(19)	0.0508(19)	0.0485(19)	-0.0156(16)	0.0266(15)	-0.0094(15)
C60	0.053(2)	0.0354(17)	0.073(2)	-0.0088(16)	0.0304(18)	-0.0003(15)
C61	0.0397(17)	0.0398(17)	0.070(2)	0.0037(16)	0.0099(16)	0.0081(14)
C62	0.0361(15)	0.0386(16)	0.0438(17)	-0.0024(13)	-0.0003(13)	0.0042(12)
C63	0.0258(13)	0.0405(16)	0.0394(15)	-0.0091(12)	0.0051(11)	-0.0077(11)
C64	0.0325(15)	0.0484(18)	0.0492(18)	0.0005(14)	0.0134(13)	-0.0024(13)
C65	0.0424(18)	0.077(3)	0.050(2)	-0.0193(19)	0.0008(15)	-0.0142(18)
C66	0.047(2)	0.047(2)	0.082(3)	0.0129(19)	0.0095(19)	-0.0064(16)
C67	0.0234(12)	0.0374(15)	0.0386(15)	-0.0001(12)	0.0026(11)	-0.0022(11)
C68	0.054(2)	0.068(2)	0.0423(18)	0.0057(17)	0.0133(15)	-0.0243(18)
C69	0.0265(15)	0.055(2)	0.078(3)	0.0095(18)	-0.0009(15)	-0.0011(14)
C70	0.0349(16)	0.0418(18)	0.074(2)	-0.0046(17)	0.0099(16)	-0.0088(13)
C71	0.109(4)	0.060(3)	0.119(5)	0.025(3)	0.070(4)	0.008(3)
C72	0.089(3)	0.068(3)	0.052(2)	0.011(2)	0.026(2)	0.015(2)
C73	0.058(2)	0.054(2)	0.0505(19)	-0.0125(17)	0.0035(17)	0.0001(17)
C3	0.0230(11)	0.0343(13)	0.0174(11)	0.0029(10)	0.0013(9)	0.0027(10)
C4	0.0269(12)	0.0353(14)	0.0257(12)	0.0071(11)	0.0038(10)	0.0014(11)

6.5 Crystal structure determination of CS_2 adduct 4

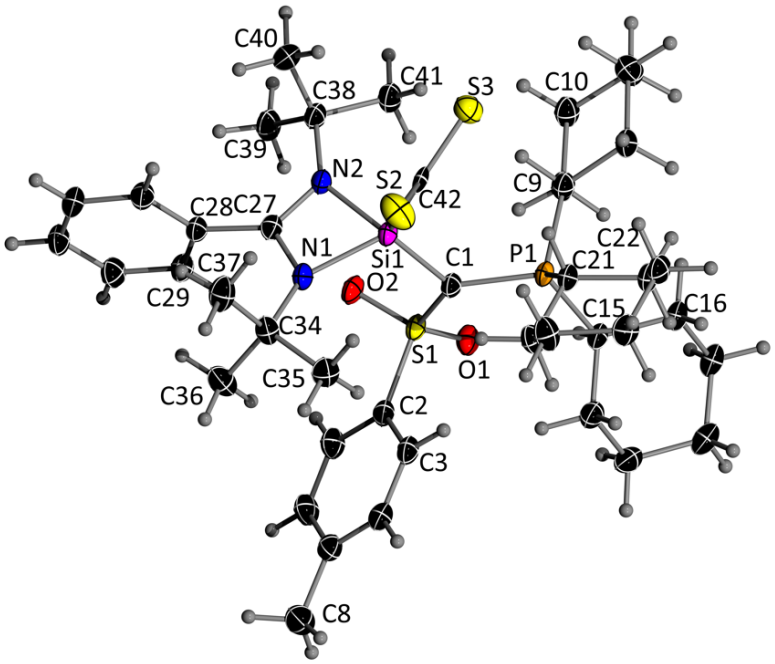


Figure S78. ORTEP of **5$_{Ts}$**. Thermal ellipsoids are drawn at the 50% probability level.

Table S10. Atomic coordinates (x 10^4) and equivalentisotropic displacement parameters ($Å^2$x 10^3) for **5_{TS}**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

atom	X	Y	Z	U(eq)
Si1	0.67462(3)	0.51472(3)	0.70011(2)	0.01928(12)
O1	0.92993(10)	0.45400(9)	0.84091(6)	0.0257(3)
O2	0.89580(9)	0.46524(9)	0.72176(6)	0.0250(3)
S1	0.86063(3)	0.43852(3)	0.78049(2)	0.02057(12)
S2	0.55229(4)	0.68093(3)	0.71635(2)	0.03213(13)
S3	0.44907(4)	0.51151(4)	0.66494(3)	0.03990(15)
P1	0.71793(3)	0.53335(3)	0.85414(2)	0.01901(12)
N1	0.67914(11)	0.42910(10)	0.63835(7)	0.0213(3)
N2	0.74208(11)	0.56280(10)	0.63991(7)	0.0210(3)
C1	0.74667(13)	0.48715(12)	0.78117(8)	0.0202(4)
C2	0.84780(14)	0.31849(12)	0.77359(8)	0.0229(4)
C12	0.82865(15)	0.83327(13)	0.89386(9)	0.0292(4)
C13	0.71676(15)	0.81867(13)	0.87200(10)	0.0284(4)
C14	0.68706(14)	0.72207(13)	0.88574(9)	0.0241(4)
C15	0.58327(14)	0.51771(12)	0.85294(8)	0.0218(4)
C16	0.54720(14)	0.54371(13)	0.91643(8)	0.0242(4)
C17	0.43317(14)	0.54094(13)	0.90489(9)	0.0265(4)
C18	0.39473(15)	0.44719(14)	0.88516(10)	0.0293(4)
C19	0.43245(15)	0.41730(15)	0.82407(10)	0.0316(4)
C20	0.54621(14)	0.42217(13)	0.83263(9)	0.0264(4)
C21	0.79406(14)	0.48906(12)	0.93014(8)	0.0221(4)
C22	0.78515(14)	0.54432(13)	0.99170(8)	0.0250(4)
C23	0.86779(15)	0.51592(14)	1.04803(9)	0.0280(4)
C24	0.86269(16)	0.41557(15)	1.06210(9)	0.0316(4)
C25	0.86449(16)	0.35958(14)	1.00103(9)	0.0305(4)
C26	0.78265(15)	0.38832(13)	0.94391(9)	0.0269(4)
C27	0.73217(13)	0.48545(12)	0.60717(8)	0.0208(4)
C28	0.77925(14)	0.46088(12)	0.55068(8)	0.0227(4)
C29	0.87431(14)	0.42231(13)	0.56433(9)	0.0251(4)
C30	0.92069(15)	0.39634(14)	0.51340(9)	0.0288(4)
C31	0.87229(16)	0.40766(14)	0.44950(9)	0.0306(4)
C32	0.77859(16)	0.44561(14)	0.43624(9)	0.0305(4)
C33	0.73173(15)	0.47351(13)	0.48675(9)	0.0265(4)
C34	0.63124(14)	0.34185(13)	0.61403(9)	0.0251(4)
C35	0.55357(16)	0.35697(16)	0.55186(10)	0.0345(5)
C36	0.57869(15)	0.30520(14)	0.66690(9)	0.0288(4)
C37	0.70966(16)	0.27339(14)	0.60155(11)	0.0343(5)
C38	0.78994(15)	0.64877(13)	0.62532(8)	0.0245(4)
C39	0.89028(16)	0.63412(14)	0.60405(10)	0.0308(4)
C40	0.71689(17)	0.69886(14)	0.57275(9)	0.0328(4)
C41	0.80826(15)	0.70336(14)	0.68838(9)	0.0284(4)
C42	0.54936(13)	0.57457(12)	0.69350(7)	0.0192(4)
C3	0.77012(14)	0.27045(13)	0.79147(8)	0.0245(4)
C4	0.76599(15)	0.17724(13)	0.78482(9)	0.0268(4)
C5	0.84054(15)	0.13038(13)	0.76138(9)	0.0276(4)
C6	0.91918(15)	0.17983(14)	0.74422(9)	0.0294(4)

C7	0.92321(14)	0.27250(14)	0.74987(9)	0.0272(4)
C8	0.83761(18)	0.02910(14)	0.75406(11)	0.0365(5)
C9	0.74722(14)	0.65481(12)	0.85253(8)	0.0220(4)
C10	0.86058(14)	0.67008(13)	0.87081(9)	0.0245(4)
C11	0.88732(15)	0.76798(13)	0.85905(9)	0.0280(4)

Table S11. Anisotropic displacement parameters(Å^2) for **5$_{TS}$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si1	0.0198(2)	0.0238(3)	0.0153(2)	-0.00060(17)	0.00619(18)	0.00082(18)
O1	0.0211(7)	0.0344(7)	0.0220(6)	-0.0012(5)	0.0047(5)	0.0028(5)
O2	0.0235(7)	0.0342(7)	0.0199(6)	0.0037(5)	0.0106(5)	0.0033(5)
S1	0.0192(2)	0.0272(2)	0.0166(2)	0.00052(16)	0.00675(16)	0.00174(17)
S2	0.0329(3)	0.0300(3)	0.0341(3)	-0.00232(19)	0.0080(2)	0.0038(2)
S3	0.0267(3)	0.0413(3)	0.0505(3)	-0.0120(2)	0.0042(2)	0.0016(2)
P1	0.0200(2)	0.0234(2)	0.0150(2)	-0.00017(16)	0.00694(17)	0.00018(17)
N1	0.0216(8)	0.0250(8)	0.0184(7)	-0.0016(6)	0.0069(6)	0.0003(6)
N2	0.0241(8)	0.0240(8)	0.0159(7)	0.0002(6)	0.0063(6)	0.0007(6)
C1	0.0209(9)	0.0242(9)	0.0167(8)	0.0005(7)	0.0067(7)	0.0027(7)
C2	0.0241(9)	0.0279(10)	0.0171(8)	-0.0002(7)	0.0052(7)	0.0034(7)
C12	0.0333(11)	0.0281(10)	0.0276(9)	-0.0029(8)	0.0089(8)	-0.0040(8)
C13	0.0316(11)	0.0260(10)	0.0285(9)	-0.0013(7)	0.0079(8)	0.0017(8)
C14	0.0242(9)	0.0280(10)	0.0210(8)	-0.0019(7)	0.0068(7)	0.0004(7)
C15	0.0218(9)	0.0269(9)	0.0179(8)	-0.0005(7)	0.0067(7)	-0.0002(7)
C16	0.0255(10)	0.0301(10)	0.0191(8)	-0.0012(7)	0.0095(7)	-0.0011(8)
C17	0.0264(10)	0.0328(10)	0.0235(9)	0.0008(8)	0.0129(8)	0.0021(8)
C18	0.0232(10)	0.0363(11)	0.0310(10)	0.0002(8)	0.0117(8)	-0.0028(8)
C19	0.0257(10)	0.0376(11)	0.0337(10)	-0.0096(9)	0.0110(8)	-0.0057(8)
C20	0.0245(10)	0.0285(10)	0.0281(9)	-0.0050(7)	0.0100(8)	-0.0010(8)
C21	0.0231(9)	0.0286(10)	0.0155(8)	0.0013(7)	0.0062(7)	0.0013(7)
C22	0.0270(10)	0.0321(10)	0.0174(8)	-0.0006(7)	0.0074(7)	-0.0006(8)
C23	0.0258(10)	0.0404(11)	0.0181(8)	0.0009(8)	0.0050(7)	-0.0030(8)
C24	0.0295(10)	0.0430(12)	0.0222(9)	0.0080(8)	0.0045(8)	-0.0012(9)
C25	0.0324(11)	0.0318(11)	0.0285(10)	0.0087(8)	0.0086(8)	0.0027(8)
C26	0.0302(10)	0.0298(10)	0.0217(9)	0.0019(7)	0.0074(8)	-0.0012(8)
C27	0.0189(9)	0.0265(9)	0.0172(8)	0.0010(7)	0.0035(7)	0.0034(7)
C28	0.0272(10)	0.0236(9)	0.0190(8)	-0.0010(7)	0.0092(7)	-0.0010(7)
C29	0.0245(9)	0.0306(10)	0.0216(9)	-0.0002(7)	0.0080(7)	0.0003(8)
C30	0.0272(10)	0.0332(10)	0.0284(10)	-0.0014(8)	0.0113(8)	0.0026(8)
C31	0.0365(11)	0.0345(11)	0.0246(9)	-0.0040(8)	0.0157(8)	0.0006(9)
C32	0.0385(11)	0.0361(11)	0.0181(9)	-0.0004(8)	0.0081(8)	0.0001(9)
C33	0.0285(10)	0.0303(10)	0.0214(9)	-0.0007(7)	0.0066(8)	0.0020(8)
C34	0.0244(9)	0.0274(9)	0.0247(9)	-0.0060(7)	0.0075(7)	-0.0035(8)
C35	0.0323(11)	0.0455(13)	0.0253(10)	-0.0048(9)	0.0041(8)	-0.0073(9)
C36	0.0261(10)	0.0314(10)	0.0299(10)	-0.0019(8)	0.0079(8)	-0.0050(8)
C37	0.0352(11)	0.0275(10)	0.0442(12)	-0.0084(9)	0.0175(9)	-0.0036(9)
C38	0.0302(10)	0.0256(9)	0.0195(8)	0.0002(7)	0.0097(7)	-0.0034(8)
C39	0.0337(11)	0.0342(11)	0.0285(10)	-0.0029(8)	0.0159(8)	-0.0069(9)
C40	0.0445(12)	0.0289(10)	0.0255(9)	0.0061(8)	0.0077(9)	0.0011(9)

C41	0.0334(11)	0.0299(10)	0.0238(9)	-0.0037(8)	0.0106(8)	-0.0076(8)
C42	0.0189(8)	0.0311(10)	0.0090(7)	0.0025(6)	0.0060(6)	0.0020(7)
C3	0.0239(9)	0.0325(10)	0.0185(8)	0.0006(7)	0.0073(7)	0.0045(8)
C4	0.0291(10)	0.0318(10)	0.0204(8)	0.0024(7)	0.0067(7)	0.0000(8)
C5	0.0317(10)	0.0295(10)	0.0207(8)	0.0003(7)	0.0024(8)	0.0050(8)
C6	0.0254(10)	0.0354(11)	0.0283(10)	-0.0045(8)	0.0073(8)	0.0078(8)
C7	0.0225(9)	0.0348(11)	0.0258(9)	-0.0021(8)	0.0083(7)	0.0028(8)
C8	0.0405(12)	0.0327(11)	0.0362(11)	-0.0032(9)	0.0068(9)	0.0034(9)
C9	0.0234(9)	0.0251(9)	0.0190(8)	-0.0003(7)	0.0076(7)	-0.0016(7)
C10	0.0228(9)	0.0289(10)	0.0231(9)	-0.0029(7)	0.0080(7)	-0.0005(7)
C11	0.0281(10)	0.0315(10)	0.0261(9)	-0.0034(8)	0.0096(8)	-0.0063(8)

6.6 Crystal structure determination of CS_2 adduct $\mathbf{5_{CN}}$

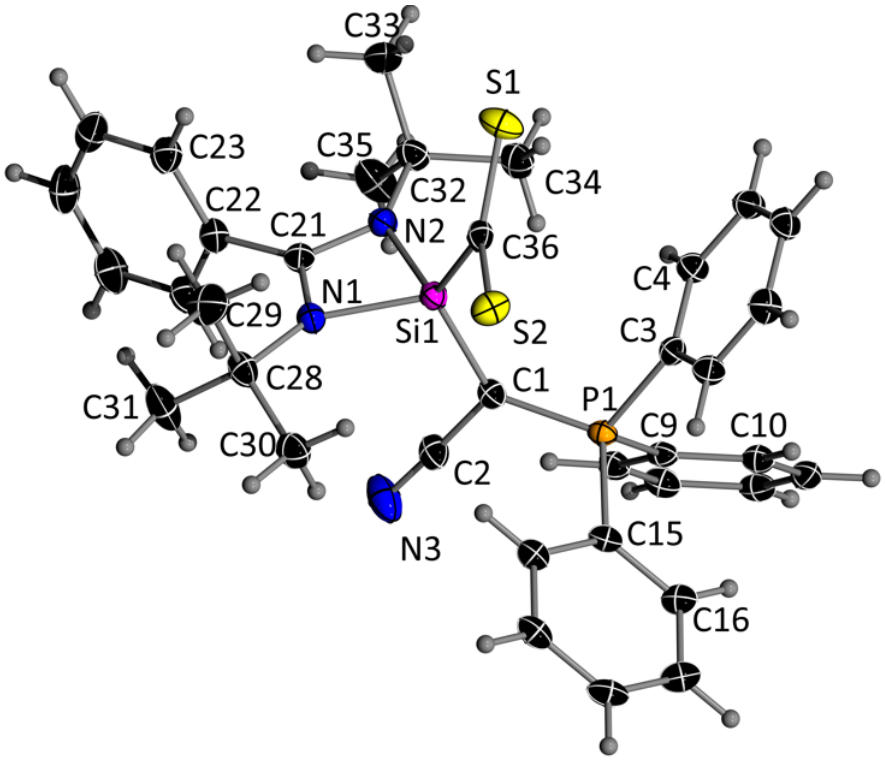


Figure S79. ORTEP of $\mathbf{5_{CN}}$. Ellipsoids are drawn at the 50% probability level.

Table S12 Atomic coordinates (x 10^4) and equivalentisotropic displacement parameters ($Å^2$x 10^3) for $\mathbf{5_{CN}}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

atom	X	Y	Z	U(eq)
Si1	0.70009(3)	0.38525(2)	0.77590(2)	0.01735(9)
N1	0.60753(10)	0.60876(9)	0.67061(10)	0.0381(3)
C1	0.74601(10)	0.49135(9)	0.74974(8)	0.0188(3)
S2	0.80233(3)	0.21770(3)	0.88505(2)	0.03057(10)
S1	0.79374(3)	0.24593(2)	0.71029(2)	0.02613(9)
P1	0.86326(2)	0.52021(2)	0.75988(2)	0.01607(9)
N2	0.56839(8)	0.37701(8)	0.71081(7)	0.0199(2)
C2	0.67092(10)	0.55675(9)	0.70627(9)	0.0236(3)

N3	0.63608(8)	0.40536(8)	0.84407(7)	0.0199(2)
C3	0.95449(9)	0.43715(9)	0.82229(8)	0.0175(2)
C4	0.97458(10)	0.42777(9)	0.90751(8)	0.0207(3)
C5	1.04629(10)	0.36598(10)	0.95715(9)	0.0227(3)
C6	1.09863(10)	0.31341(9)	0.92248(9)	0.0232(3)
C7	1.07884(10)	0.32246(10)	0.83775(9)	0.0242(3)
C8	1.00713(10)	0.38460(9)	0.78750(9)	0.0211(3)
C9	0.90616(10)	0.63038(9)	0.81345(8)	0.0179(3)
C10	1.00791(10)	0.65001(10)	0.84899(8)	0.0206(3)
C11	1.04246(10)	0.73363(10)	0.89030(8)	0.0224(3)
C12	0.97603(11)	0.79831(10)	0.89609(8)	0.0227(3)
C13	0.87520(11)	0.77938(10)	0.86122(9)	0.0225(3)
C14	0.83978(10)	0.69525(9)	0.82022(8)	0.0203(3)
C15	0.87076(10)	0.52787(9)	0.65891(8)	0.0190(3)
C16	0.94367(11)	0.57952(10)	0.64709(9)	0.0228(3)
C17	0.94906(12)	0.57854(10)	0.56918(9)	0.0261(3)
C18	0.88160(12)	0.52599(10)	0.50328(9)	0.0248(3)
C19	0.80935(11)	0.47457(10)	0.51494(9)	0.0242(3)
C20	0.80373(10)	0.47499(10)	0.59272(9)	0.0220(3)
C21	0.54855(10)	0.39625(9)	0.77774(9)	0.0198(3)
C22	0.45044(10)	0.41052(10)	0.78010(9)	0.0218(3)
C23	0.40408(11)	0.49677(10)	0.75657(10)	0.0267(3)
C24	0.31637(11)	0.51366(11)	0.76516(10)	0.0317(3)
C25	0.27599(11)	0.44530(12)	0.79738(11)	0.0333(4)
C26	0.32137(11)	0.35907(12)	0.81941(10)	0.0309(3)
C27	0.40879(10)	0.34104(10)	0.81060(9)	0.0251(3)
C28	0.50239(10)	0.34809(10)	0.62315(9)	0.0244(3)
C29	0.48379(14)	0.24393(12)	0.62389(11)	0.0389(4)
C30	0.55781(11)	0.36863(11)	0.56802(9)	0.0282(3)
C31	0.40509(12)	0.40200(14)	0.58760(11)	0.0395(4)
C32	0.66035(10)	0.43014(10)	0.93368(9)	0.0235(3)
C33	0.60267(13)	0.51547(13)	0.94012(10)	0.0364(4)
C34	0.64089(12)	0.34733(13)	0.97984(10)	0.0346(4)
C35	0.77044(11)	0.45271(11)	0.97241(9)	0.0268(3)
C36	0.77260(9)	0.27496(9)	0.79477(9)	0.0192(3)

Table S13 Anisotropic displacement parameters(Å^2) for **5$_{CN}$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si1	0.01681(17)	0.01659(17)	0.01728(17)	0.00076(12)	0.00565(14)	0.00077(12)
N1	0.0286(7)	0.0219(6)	0.0464(8)	-0.0010(6)	-0.0021(6)	0.0029(5)
C1	0.0187(6)	0.0179(6)	0.0181(6)	0.0002(5)	0.0058(5)	0.0009(5)
S2	0.0406(2)	0.02389(18)	0.02373(19)	0.00525(13)	0.00973(16)	0.00815(15)
S1	0.03141(19)	0.02181(18)	0.03011(19)	0.00003(13)	0.01765(16)	0.00120(13)
P1	0.01843(16)	0.01538(16)	0.01384(16)	-0.00019(11)	0.00609(13)	0.00013(11)
N2	0.0171(5)	0.0200(5)	0.0201(6)	-0.0004(4)	0.0052(4)	0.0000(4)
C2	0.0218(7)	0.0177(6)	0.0266(7)	-0.0019(5)	0.0050(6)	-0.0027(5)
N3	0.0195(5)	0.0216(5)	0.0184(5)	0.0014(4)	0.0073(4)	0.0012(4)
C3	0.0174(6)	0.0157(6)	0.0184(6)	-0.0011(5)	0.0065(5)	-0.0022(5)

C4	0.0220(6)	0.0218(6)	0.0189(6)	-0.0009(5)	0.0092(5)	0.0008(5)
C5	0.0249(7)	0.0231(7)	0.0187(6)	0.0025(5)	0.0074(5)	-0.0006(5)
C6	0.0209(6)	0.0187(6)	0.0259(7)	0.0027(5)	0.0056(5)	0.0010(5)
C7	0.0240(7)	0.0226(7)	0.0274(7)	-0.0018(5)	0.0120(6)	0.0032(5)
C8	0.0234(6)	0.0219(6)	0.0187(6)	-0.0009(5)	0.0094(5)	0.0004(5)
C9	0.0225(6)	0.0172(6)	0.0130(6)	-0.0001(5)	0.0063(5)	-0.0023(5)
C10	0.0225(6)	0.0221(6)	0.0174(6)	0.0004(5)	0.0082(5)	0.0001(5)
C11	0.0237(7)	0.0260(7)	0.0166(6)	-0.0004(5)	0.0074(5)	-0.0053(5)
C12	0.0325(7)	0.0192(6)	0.0160(6)	-0.0023(5)	0.0096(6)	-0.0060(5)
C13	0.0287(7)	0.0195(6)	0.0184(6)	-0.0009(5)	0.0089(6)	0.0019(5)
C14	0.0226(6)	0.0199(6)	0.0168(6)	-0.0002(5)	0.0065(5)	-0.0002(5)
C15	0.0236(6)	0.0174(6)	0.0158(6)	0.0019(5)	0.0080(5)	0.0036(5)
C16	0.0289(7)	0.0194(6)	0.0204(7)	-0.0004(5)	0.0104(6)	-0.0007(5)
C17	0.0348(8)	0.0221(7)	0.0263(7)	0.0027(6)	0.0175(6)	0.0011(6)
C18	0.0352(8)	0.0236(7)	0.0179(6)	0.0035(5)	0.0132(6)	0.0083(6)
C19	0.0260(7)	0.0257(7)	0.0168(6)	-0.0013(5)	0.0048(5)	0.0057(5)
C20	0.0223(6)	0.0229(7)	0.0186(6)	0.0002(5)	0.0064(5)	0.0018(5)
C21	0.0200(6)	0.0147(6)	0.0236(7)	0.0024(5)	0.0080(5)	0.0011(5)
C22	0.0186(6)	0.0214(6)	0.0236(7)	-0.0023(5)	0.0068(5)	-0.0003(5)
C23	0.0239(7)	0.0230(7)	0.0307(8)	0.0000(6)	0.0087(6)	0.0021(6)
C24	0.0246(7)	0.0284(8)	0.0370(9)	-0.0061(6)	0.0076(7)	0.0060(6)
C25	0.0206(7)	0.0425(9)	0.0372(9)	-0.0112(7)	0.0124(6)	-0.0008(6)
C26	0.0246(7)	0.0356(8)	0.0340(8)	-0.0060(6)	0.0134(6)	-0.0085(6)
C27	0.0229(7)	0.0233(7)	0.0275(7)	-0.0025(6)	0.0088(6)	-0.0029(5)
C28	0.0213(6)	0.0249(7)	0.0210(7)	-0.0035(5)	0.0028(5)	-0.0017(5)
C29	0.0469(10)	0.0296(8)	0.0353(9)	-0.0075(7)	0.0121(8)	-0.0154(7)
C30	0.0279(7)	0.0312(8)	0.0212(7)	-0.0031(6)	0.0059(6)	-0.0023(6)
C31	0.0246(8)	0.0576(11)	0.0266(8)	-0.0042(7)	0.0007(6)	0.0096(7)
C32	0.0237(7)	0.0286(7)	0.0180(6)	0.0004(5)	0.0085(5)	0.0020(6)
C33	0.0366(9)	0.0435(10)	0.0268(8)	-0.0067(7)	0.0106(7)	0.0128(7)
C34	0.0327(8)	0.0453(9)	0.0250(8)	0.0082(7)	0.0110(6)	-0.0050(7)
C35	0.0262(7)	0.0313(8)	0.0211(7)	-0.0036(6)	0.0079(6)	-0.0016(6)
C36	0.0158(6)	0.0164(6)	0.0230(7)	-0.0013(5)	0.0057(5)	-0.0024(5)

6.7 Crystal structure determination of Silanone 6

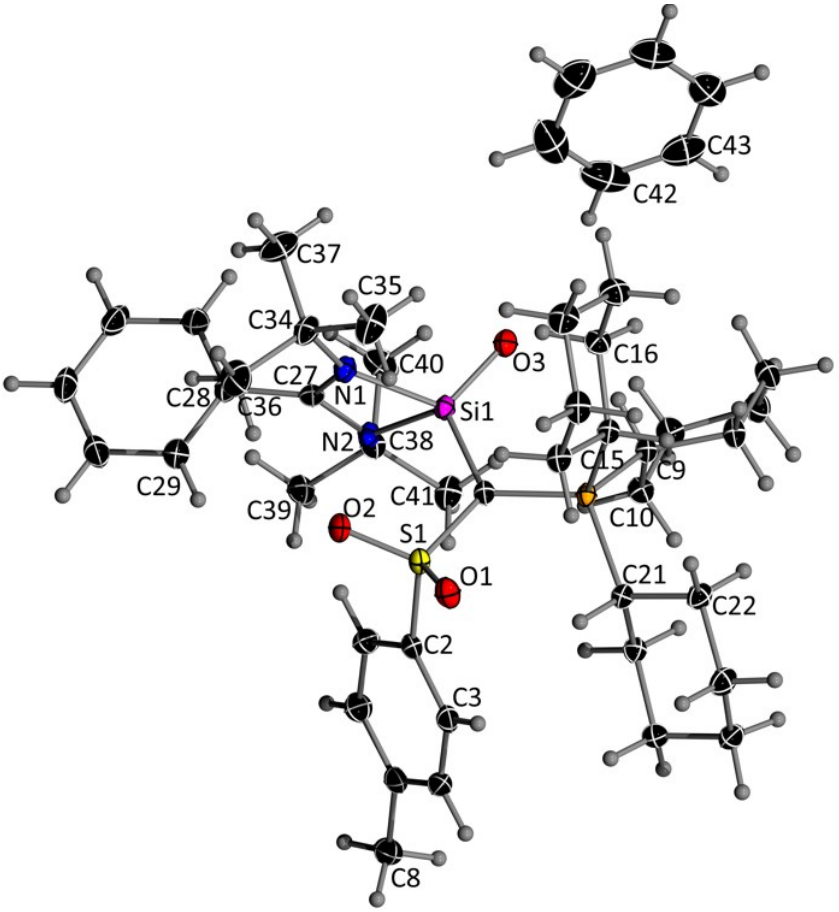


Figure S80. ORTEP of **6**. Ellipsoids are drawn at the 50% probability level.

Table S14. Atomic coordinates (x 10^4) and equivalentisotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

atom	X	Y	Z	U(eq)
S1	0.43585(3)	0.87957(2)	0.67710(2)	0.01582(8)
P1	0.51059(3)	0.65855(3)	0.62962(2)	0.01312(8)
Si1	0.45516(3)	0.66546(3)	0.80421(2)	0.01463(9)
O1	0.37936(10)	0.92562(8)	0.60505(5)	0.0213(2)
O2	0.35330(9)	0.92565(8)	0.74264(5)	0.0211(2)
O3	0.47901(9)	0.53672(8)	0.82236(5)	0.0198(2)
N1	0.30731(11)	0.74716(9)	0.86621(6)	0.0173(2)
N2	0.52755(11)	0.71552(9)	0.86671(6)	0.0160(2)
C1	0.47623(13)	0.73586(10)	0.70141(7)	0.0151(2)
C10	0.76552(13)	0.50533(11)	0.68179(8)	0.0181(3)
C11	0.82304(14)	0.38875(11)	0.73174(8)	0.0212(3)
C12	0.83895(14)	0.29613(11)	0.68986(8)	0.0218(3)
C13	0.70284(14)	0.30966(11)	0.66217(8)	0.0229(3)
C14	0.64405(14)	0.42859(11)	0.61448(8)	0.0194(3)
C15	0.35322(12)	0.63619(10)	0.61211(7)	0.0157(3)
C16	0.29227(13)	0.55951(11)	0.68074(8)	0.0186(3)
C17	0.15930(14)	0.54603(12)	0.66485(8)	0.0241(3)

C2	0.59047(13)	0.92111(10)	0.66123(7)	0.0171(3)
C18	0.05013(14)	0.65964(13)	0.64184(9)	0.0256(3)
C19	0.11178(14)	0.73236(12)	0.57186(8)	0.0221(3)
C20	0.24230(13)	0.74975(11)	0.58751(8)	0.0187(3)
C21	0.58624(13)	0.72669(10)	0.53507(7)	0.0155(2)
C22	0.57114(14)	0.68448(12)	0.46738(7)	0.0194(3)
C23	0.62909(14)	0.74920(12)	0.39113(8)	0.0225(3)
C24	0.78029(14)	0.74507(12)	0.38870(8)	0.0218(3)
C25	0.79468(14)	0.78544(11)	0.45661(7)	0.0198(3)
C26	0.74113(13)	0.71673(11)	0.53219(7)	0.0167(3)
C27	0.39733(13)	0.76044(10)	0.90186(7)	0.0163(3)
C28	0.36373(13)	0.82113(11)	0.96541(7)	0.0179(3)
C29	0.36184(14)	0.93373(12)	0.94546(8)	0.0220(3)
C30	0.33229(15)	0.99512(12)	1.00165(9)	0.0264(3)
C31	0.30734(15)	0.94347(13)	1.07794(9)	0.0287(3)
C32	0.30978(16)	0.83162(13)	1.09798(8)	0.0282(3)
C33	0.33732(14)	0.76967(12)	1.04188(8)	0.0231(3)
C34	0.15142(13)	0.79270(12)	0.87650(8)	0.0210(3)
C35	0.10573(15)	0.76433(15)	0.81275(9)	0.0332(4)
C36	0.09728(15)	0.92032(13)	0.87034(10)	0.0335(4)
C37	0.09123(15)	0.73337(15)	0.95372(9)	0.0328(4)
C38	0.65914(13)	0.66651(11)	0.90206(8)	0.0182(3)
C39	0.69255(14)	0.75313(12)	0.93162(8)	0.0218(3)
C40	0.64885(15)	0.56517(12)	0.96729(8)	0.0260(3)
C41	0.77606(14)	0.62591(13)	0.83900(8)	0.0250(3)
C42	0.3376(2)	0.33036(17)	0.84273(10)	0.0464(5)
C43	0.37049(19)	0.23376(16)	0.81526(9)	0.0391(4)
C44	0.26690(18)	0.18966(14)	0.81374(9)	0.0351(4)
C45	0.12989(18)	0.24070(15)	0.84083(10)	0.0377(4)
C46	0.0949(2)	0.33709(16)	0.86832(10)	0.0453(4)
C47	0.1993(3)	0.38263(16)	0.86906(10)	0.0514(5)
C3	0.64969(14)	0.96108(11)	0.58757(8)	0.0203(3)
C4	0.76914(14)	0.99406(11)	0.57737(8)	0.0226(3)
C5	0.82983(14)	0.98981(11)	0.63937(8)	0.0222(3)
C6	0.76618(15)	0.95235(12)	0.71289(8)	0.0246(3)
C7	0.64813(14)	0.91806(12)	0.72392(8)	0.0223(3)
C8	0.96018(15)	1.02453(12)	0.62754(9)	0.0285(3)
C9	0.62293(13)	0.51540(10)	0.66280(7)	0.0153(2)

Table S15. Anisotropic displacement parameters(Å^2) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	0.01663(15)	0.01413(15)	0.01647(16)	-0.00567(11)	-0.00192(11)	-0.00281(11)
P1	0.01193(15)	0.01421(15)	0.01396(16)	-0.00495(12)	-0.00215(11)	-0.00319(12)
Si1	0.01384(17)	0.01711(18)	0.01446(17)	-0.00591(13)	-0.00170(13)	-0.00483(13)
O1	0.0227(5)	0.0174(4)	0.0224(5)	-0.0042(4)	-0.0075(4)	-0.0017(4)
O2	0.0216(5)	0.0180(5)	0.0224(5)	-0.0087(4)	0.0018(4)	-0.0040(4)
O3	0.0230(5)	0.0201(5)	0.0179(5)	-0.0061(4)	-0.0022(4)	-0.0075(4)
N1	0.0145(5)	0.0208(5)	0.0176(5)	-0.0070(4)	-0.0010(4)	-0.0051(4)

N2	0.0154(5)	0.0182(5)	0.0160(5)	-0.0063(4)	-0.0023(4)	-0.0050(4)
C1	0.0152(6)	0.0148(6)	0.0162(6)	-0.0058(5)	-0.0021(5)	-0.0037(5)
C10	0.0162(6)	0.0182(6)	0.0208(7)	-0.0046(5)	-0.0054(5)	-0.0044(5)
C11	0.0198(6)	0.0203(7)	0.0225(7)	-0.0032(5)	-0.0075(5)	-0.0031(5)
C12	0.0200(7)	0.0175(6)	0.0243(7)	-0.0048(5)	-0.0041(5)	-0.0002(5)
C13	0.0221(7)	0.0167(6)	0.0309(8)	-0.0094(6)	-0.0042(6)	-0.0035(5)
C14	0.0179(6)	0.0192(6)	0.0230(7)	-0.0101(5)	-0.0051(5)	-0.0023(5)
C15	0.0130(6)	0.0180(6)	0.0173(6)	-0.0063(5)	-0.0028(5)	-0.0039(5)
C16	0.0168(6)	0.0216(7)	0.0196(7)	-0.0049(5)	-0.0035(5)	-0.0076(5)
C17	0.0213(7)	0.0291(7)	0.0265(7)	-0.0054(6)	-0.0052(5)	-0.0125(6)
C2	0.0198(6)	0.0128(6)	0.0188(6)	-0.0056(5)	-0.0010(5)	-0.0044(5)
C18	0.0147(6)	0.0349(8)	0.0311(8)	-0.0113(6)	-0.0044(5)	-0.0084(6)
C19	0.0167(6)	0.0251(7)	0.0257(7)	-0.0097(6)	-0.0077(5)	-0.0018(5)
C20	0.0153(6)	0.0194(6)	0.0213(7)	-0.0059(5)	-0.0049(5)	-0.0025(5)
C21	0.0155(6)	0.0163(6)	0.0146(6)	-0.0042(5)	-0.0018(5)	-0.0042(5)
C22	0.0182(6)	0.0255(7)	0.0168(6)	-0.0069(5)	-0.0017(5)	-0.0081(5)
C23	0.0247(7)	0.0285(7)	0.0153(7)	-0.0054(5)	-0.0024(5)	-0.0088(6)
C24	0.0222(7)	0.0258(7)	0.0176(7)	-0.0063(5)	0.0019(5)	-0.0094(5)
C25	0.0192(6)	0.0212(6)	0.0196(7)	-0.0048(5)	0.0000(5)	-0.0081(5)
C26	0.0159(6)	0.0179(6)	0.0171(6)	-0.0050(5)	-0.0029(5)	-0.0048(5)
C27	0.0181(6)	0.0154(6)	0.0148(6)	-0.0021(5)	-0.0013(5)	-0.0058(5)
C28	0.0141(6)	0.0222(7)	0.0190(7)	-0.0084(5)	-0.0016(5)	-0.0050(5)
C29	0.0227(7)	0.0224(7)	0.0212(7)	-0.0071(5)	-0.0021(5)	-0.0058(5)
C30	0.0259(7)	0.0225(7)	0.0336(8)	-0.0131(6)	-0.0031(6)	-0.0060(6)
C31	0.0266(7)	0.0362(8)	0.0294(8)	-0.0208(7)	0.0008(6)	-0.0093(6)
C32	0.0306(8)	0.0398(9)	0.0173(7)	-0.0112(6)	0.0028(6)	-0.0147(7)
C33	0.0238(7)	0.0258(7)	0.0223(7)	-0.0073(6)	-0.0001(5)	-0.0110(6)
C34	0.0127(6)	0.0282(7)	0.0223(7)	-0.0096(6)	-0.0003(5)	-0.0048(5)
C35	0.0163(7)	0.0532(10)	0.0345(9)	-0.0223(7)	-0.0045(6)	-0.0054(6)
C36	0.0170(7)	0.0311(8)	0.0498(10)	-0.0161(7)	0.0005(6)	-0.0014(6)
C37	0.0197(7)	0.0484(10)	0.0287(8)	-0.0046(7)	0.0001(6)	-0.0132(7)
C38	0.0165(6)	0.0200(6)	0.0200(7)	-0.0056(5)	-0.0062(5)	-0.0047(5)
C39	0.0209(7)	0.0244(7)	0.0243(7)	-0.0075(6)	-0.0062(5)	-0.0084(5)
C40	0.0288(7)	0.0221(7)	0.0285(8)	-0.0009(6)	-0.0113(6)	-0.0083(6)
C41	0.0166(6)	0.0309(8)	0.0284(8)	-0.0121(6)	-0.0051(5)	-0.0028(6)
C42	0.0689(13)	0.0527(11)	0.0309(9)	0.0128(8)	-0.0257(9)	-0.0399(10)
C43	0.0395(9)	0.0523(11)	0.0234(8)	0.0055(7)	-0.0079(7)	-0.0196(8)
C44	0.0493(10)	0.0313(8)	0.0253(8)	0.0032(6)	-0.0161(7)	-0.0136(7)
C45	0.0406(9)	0.0395(9)	0.0328(9)	0.0103(7)	-0.0166(7)	-0.0187(8)
C46	0.0480(10)	0.0452(10)	0.0275(9)	0.0048(7)	-0.0071(7)	-0.0040(8)
C47	0.0998(17)	0.0322(9)	0.0251(9)	-0.0004(7)	-0.0261(10)	-0.0173(10)
C3	0.0259(7)	0.0152(6)	0.0185(7)	-0.0054(5)	-0.0021(5)	-0.0040(5)
C4	0.0264(7)	0.0161(6)	0.0216(7)	-0.0044(5)	0.0045(5)	-0.0066(5)
C5	0.0218(7)	0.0145(6)	0.0290(7)	-0.0080(5)	0.0024(5)	-0.0051(5)
C6	0.0272(7)	0.0271(7)	0.0235(7)	-0.0071(6)	-0.0042(6)	-0.0115(6)
C7	0.0261(7)	0.0242(7)	0.0181(7)	-0.0038(5)	-0.0004(5)	-0.0115(6)
C8	0.0251(7)	0.0236(7)	0.0374(8)	-0.0100(6)	0.0039(6)	-0.0106(6)
C9	0.0147(6)	0.0150(6)	0.0164(6)	-0.0057(5)	-0.0024(5)	-0.0028(5)

6.8 Crystal structure determination of Siloxane 7

Additional information concerning the structure refinement: The unit cell contained a disordered benzene molecule. The disorder (occupancy 0.68:0.32) was solved using the PART instructions.

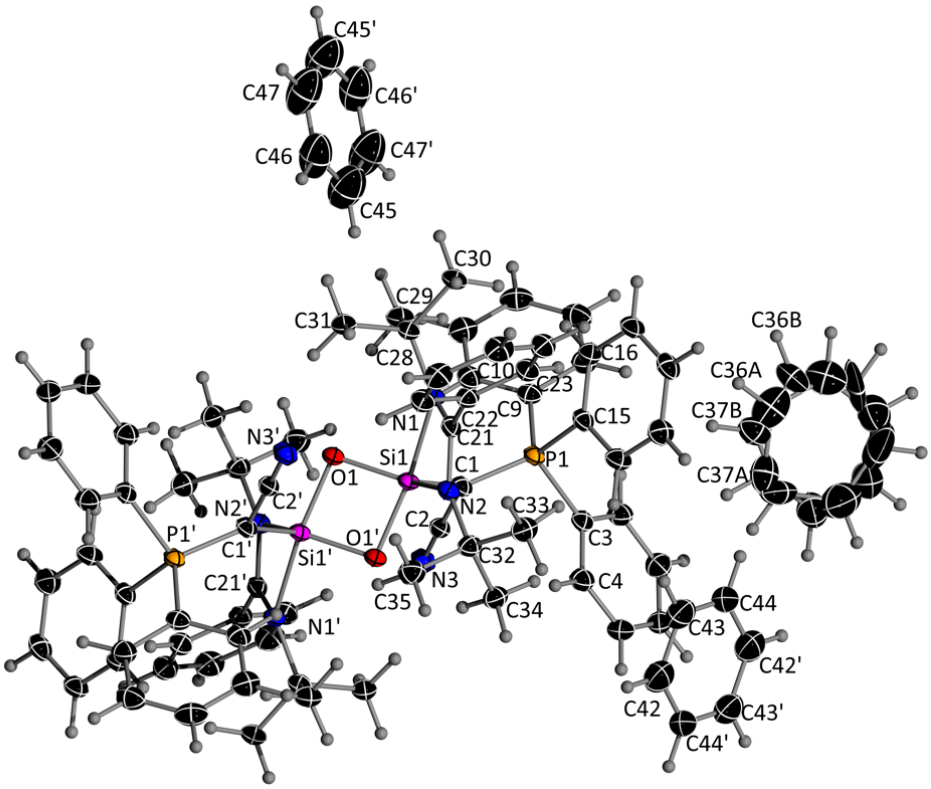


Figure S81. ORTEP of **7**. Ellipsoids are drawn at the 50% probability level.

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

Atom	X	Y	Z	U(eq)
P1	0.30797(2)	0.41919(2)	0.37431(2)	0.01924(11)
Si1	0.29340(2)	0.30185(2)	0.26924(2)	0.01769(11)
O1	0.28629(5)	0.19840(6)	0.26613(4)	0.0197(2)
N1	0.39461(6)	0.29445(7)	0.28416(5)	0.0202(3)
N2	0.33712(6)	0.36722(8)	0.22565(5)	0.0212(3)
N3	0.14752(6)	0.33155(8)	0.34768(5)	0.0257(3)
C1	0.27016(7)	0.35457(9)	0.32761(5)	0.0205(3)
C9	0.32985(7)	0.37145(10)	0.43705(6)	0.0226(3)
C10	0.31362(8)	0.28821(10)	0.44257(6)	0.0256(3)
C11	0.33029(8)	0.24768(11)	0.48897(7)	0.0319(4)
C12	0.36207(9)	0.29080(12)	0.53076(6)	0.0338(4)
C13	0.37774(9)	0.37420(11)	0.52593(6)	0.0335(4)
C2	0.20234(7)	0.34156(9)	0.33754(5)	0.0208(3)
C14	0.36311(8)	0.41444(10)	0.47920(6)	0.0282(3)
C15	0.38573(7)	0.46929(9)	0.36047(6)	0.0219(3)
C16	0.44863(7)	0.44371(10)	0.38492(6)	0.0245(3)
C17	0.50720(8)	0.48759(10)	0.37766(6)	0.0273(3)
C18	0.50387(8)	0.55685(10)	0.34626(6)	0.0281(3)

C19	0.44163(8)	0.58161(10)	0.32125(6)	0.0297(3)
C20	0.38282(8)	0.53828(10)	0.32817(6)	0.0268(3)
C21	0.40002(7)	0.33940(9)	0.24295(6)	0.0207(3)
C22	0.46239(7)	0.35494(9)	0.21718(6)	0.0228(3)
C23	0.51074(8)	0.41284(10)	0.23707(6)	0.0266(3)
C24	0.56668(8)	0.42895(10)	0.21137(7)	0.0310(4)
C25	0.57447(8)	0.38782(11)	0.16613(7)	0.0336(4)
C26	0.52681(8)	0.32914(11)	0.14654(7)	0.0319(4)
C27	0.47047(8)	0.31254(10)	0.17195(6)	0.0258(3)
C28	0.44235(7)	0.22953(9)	0.30688(6)	0.0225(3)
C29	0.41520(8)	0.20018(10)	0.35592(6)	0.0273(3)
C30	0.51515(8)	0.26188(10)	0.32085(7)	0.0281(3)
C31	0.44391(8)	0.15627(10)	0.26989(6)	0.0262(3)
C32	0.31445(8)	0.42771(9)	0.18451(6)	0.0239(3)
C33	0.36939(8)	0.49147(10)	0.17474(7)	0.0303(4)
C34	0.29117(9)	0.37987(11)	0.13518(6)	0.0309(4)
C35	0.25426(8)	0.47634(10)	0.20135(6)	0.0273(3)
C42	0.24494(13)	0.71247(13)	0.20287(9)	0.0564(6)
C43	0.30377(11)	0.70422(13)	0.23638(10)	0.0518(5)
C44	0.30801(11)	0.74163(12)	0.28344(10)	0.0543(6)
C45	0.44863(18)	0.04760(17)	0.47509(10)	0.0750(8)
C46	0.49073(17)	0.00323(16)	0.44739(9)	0.0698(7)
C47	0.54163(18)	-0.04430(17)	0.47197(10)	0.0747(8)
C3	0.24913(7)	0.50399(9)	0.38346(6)	0.0216(3)
C4	0.21342(8)	0.53959(10)	0.33970(6)	0.0263(3)
C5	0.17125(8)	0.60753(10)	0.34423(6)	0.0297(3)
C6	0.16312(8)	0.63940(10)	0.39215(7)	0.0291(3)
C7	0.19613(8)	0.60264(11)	0.43563(7)	0.0304(3)
C8	0.23951(8)	0.53536(10)	0.43130(6)	0.0268(3)
C36A	0.4231(4)	0.6724(2)	0.4570(3)	0.059(2)
C37A	0.3597(3)	0.6974(3)	0.43377(18)	0.0463(18)
C38A	0.32850(15)	0.7672(4)	0.45171(18)	0.0532(14)
C39A	0.3607(2)	0.8120(2)	0.4928(2)	0.0628(16)
C40A	0.4241(2)	0.7870(4)	0.51606(13)	0.0605(17)
C41A	0.45530(17)	0.7172(5)	0.4981(2)	0.056(2)
C36B	0.4491(3)	0.6796(6)	0.4836(4)	0.043(3)
C41B	0.4498(8)	0.7523(8)	0.5123(3)	0.074(6)
C40B	0.3978(11)	0.8101(4)	0.5022(5)	0.086(7)
C39B	0.3451(7)	0.7953(7)	0.4635(7)	0.076(5)
C38B	0.3444(4)	0.7226(9)	0.4348(5)	0.050(4)
C37B	0.3964(6)	0.6647(5)	0.4448(4)	0.042(3)

Table S17. Anisotropic displacement parameters(Å^2) for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P1	0.01341(18)	0.0218(2)	0.0223(2)	-0.00203(13)	0.00133(13)	-0.00058(13)
Si1	0.01178(19)	0.0198(2)	0.0214(2)	-0.00119(14)	0.00145(14)	-0.00063(14)
O1	0.0136(5)	0.0214(5)	0.0236(5)	-0.0009(4)	0.0004(4)	-0.0003(4)

N1	0.0134(6)	0.0215(6)	0.0257(6)	-0.0017(5)	0.0016(5)	-0.0002(5)
N2	0.0152(6)	0.0229(6)	0.0256(6)	-0.0002(5)	0.0024(5)	-0.0009(5)
N3	0.0179(6)	0.0300(7)	0.0292(7)	-0.0043(5)	0.0029(5)	-0.0013(5)
C1	0.0142(7)	0.0234(7)	0.0236(7)	-0.0024(6)	0.0012(5)	-0.0019(5)
C9	0.0171(7)	0.0268(7)	0.0241(7)	-0.0005(6)	0.0032(5)	0.0024(6)
C10	0.0195(7)	0.0295(8)	0.0283(8)	-0.0013(6)	0.0045(6)	-0.0005(6)
C11	0.0279(9)	0.0339(9)	0.0346(9)	0.0066(7)	0.0073(7)	0.0011(7)
C12	0.0302(9)	0.0444(10)	0.0270(8)	0.0074(7)	0.0038(7)	0.0077(7)
C13	0.0302(9)	0.0429(10)	0.0260(8)	-0.0044(7)	-0.0019(7)	0.0055(7)
C2	0.0178(7)	0.0217(7)	0.0224(7)	-0.0031(6)	0.0002(5)	0.0007(5)
C14	0.0249(8)	0.0299(8)	0.0293(8)	-0.0037(6)	0.0009(6)	0.0028(6)
C15	0.0163(7)	0.0250(7)	0.0245(7)	-0.0049(6)	0.0027(5)	-0.0021(6)
C16	0.0192(7)	0.0243(7)	0.0297(8)	-0.0026(6)	0.0013(6)	0.0005(6)
C17	0.0153(7)	0.0317(8)	0.0341(8)	-0.0055(7)	-0.0001(6)	0.0002(6)
C18	0.0189(7)	0.0328(8)	0.0329(8)	-0.0060(7)	0.0050(6)	-0.0068(6)
C19	0.0246(8)	0.0310(8)	0.0338(9)	0.0040(7)	0.0052(6)	-0.0035(6)
C20	0.0174(7)	0.0323(8)	0.0301(8)	0.0013(6)	0.0008(6)	-0.0010(6)
C21	0.0159(7)	0.0203(7)	0.0261(7)	-0.0046(6)	0.0028(6)	-0.0017(5)
C22	0.0162(7)	0.0228(7)	0.0296(8)	0.0023(6)	0.0036(6)	0.0006(6)
C23	0.0195(7)	0.0259(8)	0.0346(8)	-0.0006(6)	0.0033(6)	-0.0009(6)
C24	0.0189(8)	0.0272(8)	0.0472(10)	0.0035(7)	0.0048(7)	-0.0033(6)
C25	0.0213(8)	0.0358(9)	0.0458(10)	0.0067(8)	0.0130(7)	-0.0007(7)
C26	0.0275(8)	0.0350(9)	0.0351(9)	0.0000(7)	0.0118(7)	0.0031(7)
C27	0.0203(7)	0.0260(8)	0.0315(8)	-0.0003(6)	0.0044(6)	-0.0007(6)
C28	0.0146(7)	0.0241(7)	0.0282(8)	-0.0001(6)	0.0008(6)	0.0006(6)
C29	0.0194(7)	0.0324(8)	0.0298(8)	0.0031(6)	0.0010(6)	0.0033(6)
C30	0.0161(7)	0.0298(8)	0.0373(9)	-0.0020(7)	-0.0017(6)	0.0005(6)
C31	0.0198(7)	0.0260(8)	0.0325(8)	-0.0018(6)	0.0012(6)	0.0037(6)
C32	0.0203(7)	0.0231(7)	0.0283(8)	0.0036(6)	0.0032(6)	0.0004(6)
C33	0.0252(8)	0.0283(8)	0.0381(9)	0.0073(7)	0.0069(7)	-0.0004(6)
C34	0.0320(9)	0.0322(9)	0.0279(8)	0.0019(7)	0.0007(7)	0.0025(7)
C35	0.0225(8)	0.0246(8)	0.0350(8)	0.0039(6)	0.0040(6)	0.0027(6)
C42	0.0700(15)	0.0368(11)	0.0578(13)	0.0014(10)	-0.0110(11)	0.0063(10)
C43	0.0453(12)	0.0324(10)	0.0761(15)	0.0069(10)	-0.0001(10)	0.0031(8)
C44	0.0463(12)	0.0324(10)	0.0766(16)	0.0036(10)	-0.0241(11)	-0.0003(9)
C45	0.109(2)	0.0569(15)	0.0586(15)	0.0038(12)	0.0099(15)	0.0102(15)
C46	0.116(2)	0.0500(13)	0.0420(12)	-0.0030(10)	0.0058(13)	-0.0041(14)
C47	0.118(2)	0.0527(14)	0.0560(15)	-0.0036(12)	0.0223(15)	0.0092(15)
C3	0.0145(7)	0.0228(7)	0.0277(7)	-0.0025(6)	0.0029(5)	-0.0022(5)
C4	0.0213(7)	0.0297(8)	0.0278(8)	-0.0026(6)	0.0015(6)	0.0017(6)
C5	0.0218(8)	0.0307(8)	0.0352(9)	0.0013(7)	-0.0026(6)	0.0041(6)
C6	0.0194(7)	0.0262(8)	0.0412(9)	-0.0046(7)	0.0016(6)	0.0032(6)
C7	0.0255(8)	0.0340(9)	0.0320(8)	-0.0080(7)	0.0046(6)	0.0038(7)
C8	0.0224(7)	0.0303(8)	0.0275(8)	-0.0017(6)	0.0018(6)	0.0032(6)
C36A	0.073(6)	0.052(2)	0.057(5)	0.007(2)	0.039(4)	0.007(3)
C37A	0.052(4)	0.039(3)	0.052(3)	-0.003(2)	0.021(3)	-0.010(3)
C38A	0.051(3)	0.050(3)	0.058(3)	-0.009(2)	0.006(2)	-0.005(2)
C39A	0.063(4)	0.054(3)	0.069(3)	-0.015(2)	-0.002(3)	-0.002(2)
C40A	0.054(3)	0.059(5)	0.069(3)	-0.010(3)	0.008(2)	-0.010(3)

C41A	0.048(3)	0.077(6)	0.047(3)	0.002(3)	0.014(2)	0.002(3)
C36B	0.031(4)	0.061(7)	0.036(6)	-0.007(5)	-0.003(4)	-0.009(4)
C41B	0.122(15)	0.052(9)	0.044(6)	-0.020(6)	-0.007(8)	-0.047(9)
C40B	0.13(2)	0.037(5)	0.093(11)	-0.017(6)	0.013(11)	0.017(9)
C39B	0.057(7)	0.062(9)	0.108(15)	0.013(9)	0.009(8)	0.008(7)
C38B	0.030(4)	0.048(8)	0.069(9)	0.027(6)	-0.003(4)	0.002(5)
C37B	0.039(7)	0.050(5)	0.034(4)	0.008(3)	-0.001(4)	-0.005(5)

6.8 Crystal structure determination of Carbonate Complex 8

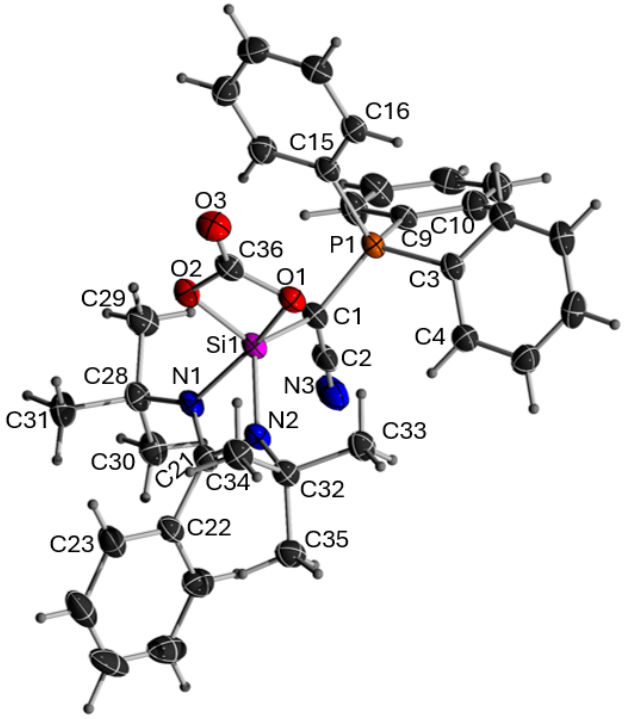


Figure S82. ORTEP of **8**. Ellipsoids are drawn at the 50% probability level.

Table S18. Atomic coordinates (x 104) and equivalentisotropic displacement parameters (Å2x 103) for **8** U(eq) is defined as one third of the trace of the orthogonalized Uij tensor for all atoms.

Atom	x	y	z	U(eq)
Si(1)	8582(1)	5765(1)	6885(1)	22(1)
O(1)	9583(1)	5691(1)	7911(1)	26(1)
N(1)	8022(1)	5804(1)	5632(1)	24(1)
C(1)	7263(1)	5821(1)	7381(1)	24(1)
C(3)	7666(1)	6322(1)	9290(1)	24(1)
C(4)	7883(1)	7006(1)	8929(1)	30(1)
C(5)	8250(1)	7592(1)	9494(1)	36(1)
C(6)	8411(1)	7501(1)	10422(1)	34(1)
C(7)	8190(1)	6827(1)	10790(1)	33(1)
C(8)	7809(1)	6239(1)	10234(1)	28(1)
C(9)	5652(1)	5472(1)	8602(1)	25(1)

C(10)	5160(1)	5799(1)	9299(1)	30(1)
C(11)	4000(1)	5709(1)	9344(1)	33(1)
C(12)	3322(1)	5303(1)	8693(1)	33(1)
C(13)	3811(1)	4955(1)	8018(1)	36(1)
C(14)	4971(1)	5038(1)	7968(1)	34(1)
P(1)	7153(1)	5603(1)	8493(1)	21(1)
C(15)	7875(1)	4733(1)	8801(1)	24(1)
C(16)	8628(1)	4620(1)	9599(1)	26(1)
C(2)	6301(1)	6168(1)	6891(1)	28(1)
O(3)	10706(1)	4660(1)	7976(1)	35(1)
N(3)	5520(1)	6452(1)	6476(1)	43(1)
C(17)	9089(1)	3926(1)	9804(1)	30(1)
C(18)	8818(1)	3341(1)	9218(1)	32(1)
C(19)	8087(1)	3452(1)	8416(1)	33(1)
C(20)	7618(1)	4143(1)	8207(1)	31(1)
C(21)	8663(1)	6385(1)	5540(1)	24(1)
C(22)	8830(1)	6758(1)	4680(1)	28(1)
C(23)	9728(1)	6543(1)	4225(1)	36(1)
C(24)	9902(2)	6912(1)	3437(1)	49(1)
C(25)	9200(2)	7485(1)	3118(1)	54(1)
C(26)	8293(2)	7689(1)	3560(1)	49(1)
C(27)	8098(2)	7325(1)	4343(1)	36(1)
C(28)	7311(1)	5357(1)	4929(1)	28(1)
C(29)	6806(2)	4728(1)	5428(1)	38(1)
O(2)	9308(1)	4946(1)	6795(1)	26(1)
N(2)	9169(1)	6573(1)	6384(1)	24(1)
C(30)	6341(1)	5818(1)	4420(1)	34(1)
C(31)	8055(1)	5033(1)	4266(1)	35(1)
C(32)	10105(1)	7115(1)	6661(1)	26(1)
C(33)	10006(1)	7370(1)	7625(1)	31(1)
C(34)	11255(1)	6733(1)	6629(1)	32(1)
C(35)	10018(1)	7804(1)	6061(1)	33(1)
C(36)	9961(1)	5052(1)	7618(1)	27(1)

Table S19. Anisotropic displacement parameters($Å^2$) for **8**The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

Si(1)	20(1)	28(1)	17(1)	0(1)	3(1)	-2(1)
O(1)	25(1)	32(1)	21(1)	0(1)	3(1)	-3(1)
N(1)	23(1)	31(1)	18(1)	-1(1)	2(1)	-2(1)
C(1)	22(1)	30(1)	19(1)	1(1)	4(1)	0(1)
C(3)	20(1)	29(1)	23(1)	-2(1)	4(1)	0(1)
C(4)	32(1)	30(1)	28(1)	0(1)	8(1)	0(1)
C(5)	40(1)	28(1)	42(1)	-4(1)	14(1)	-5(1)
C(6)	25(1)	36(1)	40(1)	-14(1)	6(1)	-2(1)
C(7)	30(1)	43(1)	26(1)	-8(1)	3(1)	2(1)
C(8)	28(1)	32(1)	25(1)	-1(1)	5(1)	0(1)
C(9)	21(1)	31(1)	23(1)	3(1)	4(1)	-2(1)
C(10)	26(1)	34(1)	30(1)	-2(1)	7(1)	-2(1)
C(11)	29(1)	38(1)	36(1)	1(1)	11(1)	0(1)
C(12)	23(1)	41(1)	36(1)	10(1)	6(1)	-3(1)
C(13)	26(1)	51(1)	29(1)	-2(1)	-1(1)	-10(1)
C(14)	28(1)	47(1)	26(1)	-6(1)	4(1)	-5(1)
P(1)	19(1)	27(1)	18(1)	0(1)	4(1)	-2(1)
C(15)	20(1)	29(1)	23(1)	0(1)	6(1)	-3(1)
C(16)	22(1)	33(1)	24(1)	-1(1)	5(1)	-2(1)
C(2)	29(1)	37(1)	21(1)	1(1)	8(1)	3(1)
O(3)	26(1)	42(1)	35(1)	6(1)	-1(1)	3(1)
N(3)	40(1)	60(1)	30(1)	8(1)	8(1)	20(1)
C(17)	22(1)	39(1)	29(1)	6(1)	3(1)	1(1)
C(18)	25(1)	31(1)	41(1)	6(1)	9(1)	2(1)
C(19)	34(1)	30(1)	36(1)	-4(1)	7(1)	-2(1)
C(20)	31(1)	33(1)	27(1)	-1(1)	1(1)	-2(1)
C(21)	21(1)	30(1)	21(1)	0(1)	4(1)	2(1)
C(22)	31(1)	33(1)	19(1)	0(1)	3(1)	-5(1)
C(23)	40(1)	44(1)	27(1)	-4(1)	11(1)	-7(1)
C(24)	60(1)	63(1)	28(1)	-9(1)	19(1)	-25(1)
C(25)	85(2)	53(1)	21(1)	6(1)	0(1)	-32(1)
C(26)	71(1)	38(1)	31(1)	7(1)	-15(1)	-12(1)
C(27)	42(1)	35(1)	28(1)	2(1)	-5(1)	-2(1)
C(28)	27(1)	34(1)	21(1)	-4(1)	0(1)	-3(1)
C(29)	43(1)	40(1)	29(1)	-2(1)	-1(1)	-14(1)
O(2)	23(1)	33(1)	22(1)	-1(1)	2(1)	1(1)
N(2)	24(1)	31(1)	19(1)	0(1)	4(1)	-4(1)

C(30)	28(1)	45(1)	27(1)	-5(1)	-2(1)	0(1)
C(31)	35(1)	41(1)	28(1)	-9(1)	2(1)	2(1)
C(32)	24(1)	31(1)	24(1)	-1(1)	3(1)	-6(1)
C(33)	33(1)	35(1)	26(1)	-4(1)	5(1)	-6(1)
C(34)	25(1)	40(1)	32(1)	-1(1)	5(1)	-4(1)
C(35)	36(1)	33(1)	29(1)	2(1)	4(1)	-6(1)
C(36)	21(1)	35(1)	24(1)	2(1)	4(1)	-4(1)

6.9 Crystal structure determination of Silazine 9_{Ts}

Additional information concerning the structure refinement: The unit cell contained a disordered toluene molecule. The disorder (occupancy 0.57:0.43) was solved using the PART instructions.

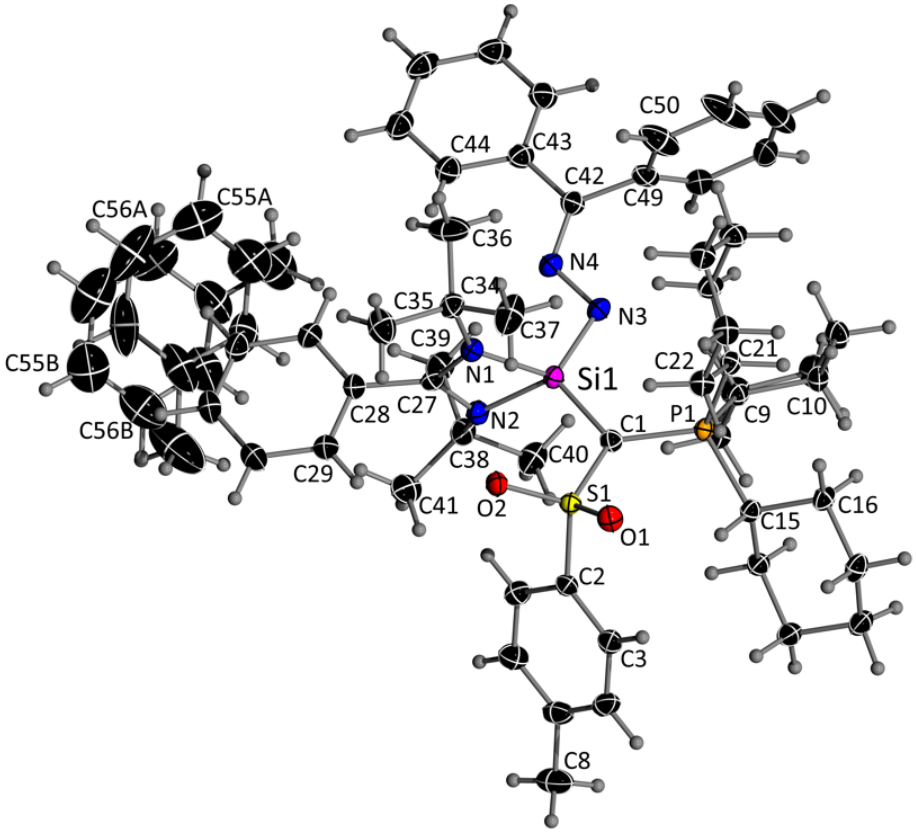


Figure S83. ORTEP of 9_{Ts}. Ellipsoids are drawn at the 50% probability level.

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 9_{Ts}. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

Atom	X	Y	Z	U(eq)
Si1	0.35941(4)	0.68631(3)	0.24412(2)	0.01783(9)
O1	0.35264(10)	0.90943(8)	0.07104(5)	0.0228(2)
N2	0.40429(12)	0.75420(10)	0.30526(6)	0.0215(3)
S1	0.38810(3)	0.88173(3)	0.13662(2)	0.01788(9)

P1	0.46789(3)	0.66631(3)	0.11205(2)	0.01544(9)
O2	0.29698(10)	0.91998(8)	0.17905(5)	0.0225(2)
N1	0.20449(12)	0.74534(10)	0.27100(6)	0.0206(3)
N3	0.36445(13)	0.55149(10)	0.26123(6)	0.0218(3)
N4	0.32025(12)	0.51525(10)	0.32206(6)	0.0220(3)
C3	0.61255(16)	0.99462(11)	0.08791(7)	0.0246(3)
C4	0.72983(16)	1.04699(12)	0.09322(8)	0.0291(4)
C1	0.41602(14)	0.74562(11)	0.16391(7)	0.0181(3)
C2	0.53934(15)	0.95014(11)	0.14107(7)	0.0206(3)
C5	0.77429(16)	1.05799(12)	0.15088(8)	0.0294(4)
C6	0.69660(17)	1.01610(13)	0.20334(8)	0.0299(4)
C7	0.58057(16)	0.96197(12)	0.19879(7)	0.0259(3)
C8	0.90332(18)	1.11320(14)	0.15662(10)	0.0406(4)
C9	0.56449(14)	0.54724(11)	0.15407(6)	0.0177(3)
C10	0.68409(15)	0.56798(12)	0.19225(7)	0.0214(3)
C11	0.73162(17)	0.46219(13)	0.23573(7)	0.0273(3)
C12	0.77288(18)	0.37901(13)	0.19866(8)	0.0315(4)
C13	0.66011(17)	0.36225(12)	0.15603(7)	0.0272(3)
C14	0.60901(15)	0.46893(11)	0.11369(7)	0.0206(3)
C15	0.32646(14)	0.61132(11)	0.07765(6)	0.0180(3)
C16	0.25041(15)	0.52508(12)	0.12460(7)	0.0225(3)
C17	0.13388(15)	0.48510(13)	0.09274(8)	0.0263(3)
C18	0.03888(15)	0.57695(13)	0.06012(8)	0.0265(3)
C19	0.11597(15)	0.65868(13)	0.01222(7)	0.0258(3)
C20	0.23118(15)	0.70233(12)	0.04294(7)	0.0221(3)
C21	0.56352(14)	0.74199(11)	0.04438(6)	0.0185(3)
C22	0.70997(14)	0.75966(11)	0.06025(7)	0.0203(3)
C23	0.77840(15)	0.83427(12)	0.00498(7)	0.0246(3)
C24	0.77529(16)	0.78945(13)	-0.05319(7)	0.0268(3)
C25	0.63285(16)	0.76544(13)	-0.06855(7)	0.0247(3)
C26	0.56222(15)	0.69306(12)	-0.01319(7)	0.0213(3)
C27	0.27325(15)	0.77903(11)	0.31310(7)	0.0204(3)
C28	0.22110(15)	0.84396(12)	0.35643(7)	0.0236(3)
C29	0.22828(18)	0.95528(13)	0.33496(8)	0.0321(4)
C30	0.1811(2)	1.02180(14)	0.37188(9)	0.0394(4)
C31	0.12876(19)	0.97833(14)	0.43028(9)	0.0372(4)
C32	0.12201(17)	0.86803(14)	0.45194(8)	0.0316(4)
C33	0.16745(16)	0.80031(13)	0.41476(7)	0.0252(3)
C34	0.05843(15)	0.74771(12)	0.25890(7)	0.0237(3)
C35	0.00265(18)	0.64481(15)	0.29960(11)	0.0436(5)
C36	0.04166(18)	0.74965(19)	0.19033(9)	0.0452(5)
C37	-0.01639(18)	0.84594(14)	0.27201(9)	0.0368(4)
C38	0.51308(15)	0.74007(13)	0.35296(7)	0.0256(3)
C39	0.54219(19)	0.84530(15)	0.37106(8)	0.0349(4)
C40	0.47683(17)	0.65475(14)	0.41172(8)	0.0303(4)
C41	0.63697(16)	0.70004(16)	0.32303(8)	0.0338(4)
C42	0.29243(15)	0.41459(12)	0.34089(7)	0.0224(3)
C43	0.24544(15)	0.37667(12)	0.40583(7)	0.0240(3)
C44	0.20012(16)	0.44949(13)	0.44084(8)	0.0282(3)

C45	0.15430(17)	0.41344(15)	0.50133(8)	0.0322(4)
C46	0.15161(18)	0.30450(15)	0.52890(8)	0.0343(4)
C47	0.19704(19)	0.23166(14)	0.49529(8)	0.0343(4)
C48	0.24251(17)	0.26700(13)	0.43455(8)	0.0298(4)
C49	0.29999(18)	0.33672(12)	0.29960(7)	0.0284(4)
C50	0.4135(2)	0.27270(14)	0.29687(9)	0.0404(4)
C51	0.4144(3)	0.19651(16)	0.26077(11)	0.0601(7)
C52	0.3032(4)	0.18472(17)	0.22753(9)	0.0682(9)
C53	0.1917(3)	0.24898(17)	0.22908(10)	0.0667(8)
C54	0.1882(2)	0.32505(14)	0.26508(9)	0.0451(5)
C55A	0.3259(10)	0.8287(10)	0.5812(6)	0.059(2)
C56A	0.3563(5)	0.7300(5)	0.5655(3)	0.0484(12)
C57A	0.2662(5)	0.6480(5)	0.5788(2)	0.0557(14)
C58A	0.1478(5)	0.6552(5)	0.6064(2)	0.0624(16)
C59A	0.1142(8)	0.7520(11)	0.6245(3)	0.076(3)
C60A	0.2046(7)	0.8347(6)	0.6123(3)	0.071(2)
C61A	0.4233(8)	0.9179(5)	0.5624(4)	0.104(3)
C55B	0.2939(11)	0.7186(5)	0.5909(3)	0.057(2)
C56B	0.1686(10)	0.7291(10)	0.6223(5)	0.061(3)
C57B	0.1341(13)	0.8284(10)	0.6337(4)	0.079(3)
C58B	0.2124(8)	0.9166(7)	0.6140(3)	0.071(2)
C59B	0.3278(10)	0.9079(7)	0.5834(4)	0.073(2)
C60B	0.3641(15)	0.8042(14)	0.5750(8)	0.060(3)
C61B	0.3343(13)	0.6135(7)	0.5820(3)	0.076(3)

Table S21. Anisotropic displacement parameters(Å^2) for **9$_{Ts}$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si1	0.01913(19)	0.01897(19)	0.01566(19)	-0.00452(15)	0.00133(14)	-0.00180(14)
O1	0.0285(5)	0.0201(5)	0.0182(5)	-0.0020(4)	-0.0023(4)	0.0031(4)
N2	0.0223(6)	0.0250(6)	0.0187(6)	-0.0076(5)	0.0015(5)	-0.0039(5)
S1	0.02124(17)	0.01539(16)	0.01652(17)	-0.00302(13)	0.00162(13)	0.00023(12)
P1	0.01628(17)	0.01675(17)	0.01343(17)	-0.00392(13)	-0.00019(13)	-0.00012(13)
O2	0.0256(5)	0.0188(5)	0.0233(5)	-0.0059(4)	0.0052(4)	0.0017(4)
N1	0.0215(6)	0.0211(6)	0.0200(6)	-0.0062(5)	0.0032(5)	-0.0026(5)
N3	0.0254(6)	0.0224(6)	0.0173(6)	-0.0037(5)	0.0033(5)	-0.0024(5)
N4	0.0244(6)	0.0223(6)	0.0189(6)	-0.0039(5)	0.0022(5)	-0.0021(5)
C3	0.0306(8)	0.0170(7)	0.0246(8)	-0.0023(6)	0.0046(6)	0.0011(6)
C4	0.0296(8)	0.0198(7)	0.0345(9)	0.0001(6)	0.0097(7)	-0.0016(6)
C1	0.0208(7)	0.0164(7)	0.0168(7)	-0.0034(5)	-0.0004(5)	0.0002(5)
C2	0.0236(7)	0.0143(6)	0.0230(8)	-0.0030(6)	0.0028(6)	0.0003(5)
C5	0.0251(8)	0.0183(7)	0.0426(10)	-0.0025(7)	0.0022(7)	-0.0016(6)
C6	0.0306(9)	0.0284(8)	0.0312(9)	-0.0071(7)	-0.0020(7)	-0.0053(7)
C7	0.0281(8)	0.0250(8)	0.0234(8)	-0.0030(6)	0.0030(6)	-0.0041(6)
C8	0.0306(9)	0.0307(9)	0.0581(13)	-0.0046(8)	0.0014(8)	-0.0091(7)
C9	0.0196(7)	0.0175(7)	0.0156(7)	-0.0033(5)	0.0008(5)	0.0000(5)
C10	0.0218(7)	0.0236(7)	0.0185(7)	-0.0042(6)	-0.0031(6)	0.0004(6)
C11	0.0297(8)	0.0289(8)	0.0214(8)	-0.0019(6)	-0.0059(6)	0.0020(6)

C12	0.0361(9)	0.0274(8)	0.0269(9)	0.0001(7)	-0.0046(7)	0.0109(7)
C13	0.0354(9)	0.0204(7)	0.0248(8)	-0.0043(6)	0.0018(7)	0.0045(6)
C14	0.0229(7)	0.0203(7)	0.0191(7)	-0.0064(6)	0.0009(6)	0.0025(6)
C15	0.0178(7)	0.0214(7)	0.0158(7)	-0.0065(6)	-0.0009(5)	-0.0005(5)
C16	0.0198(7)	0.0266(7)	0.0212(8)	-0.0053(6)	-0.0006(6)	-0.0038(6)
C17	0.0226(8)	0.0300(8)	0.0270(8)	-0.0074(7)	-0.0013(6)	-0.0065(6)
C18	0.0184(7)	0.0373(9)	0.0272(8)	-0.0142(7)	-0.0032(6)	-0.0020(6)
C19	0.0222(8)	0.0313(8)	0.0251(8)	-0.0094(6)	-0.0064(6)	0.0025(6)
C20	0.0204(7)	0.0248(7)	0.0212(7)	-0.0056(6)	-0.0036(6)	0.0012(6)
C21	0.0198(7)	0.0194(7)	0.0158(7)	-0.0032(5)	0.0015(5)	-0.0001(5)
C22	0.0203(7)	0.0203(7)	0.0200(7)	-0.0043(6)	0.0012(6)	-0.0006(5)
C23	0.0224(7)	0.0240(7)	0.0266(8)	-0.0045(6)	0.0053(6)	-0.0026(6)
C24	0.0265(8)	0.0286(8)	0.0243(8)	-0.0045(6)	0.0082(6)	-0.0016(6)
C25	0.0278(8)	0.0288(8)	0.0159(7)	-0.0025(6)	0.0036(6)	0.0020(6)
C26	0.0222(7)	0.0264(7)	0.0154(7)	-0.0055(6)	0.0015(6)	-0.0013(6)
C27	0.0260(8)	0.0182(7)	0.0162(7)	-0.0018(5)	0.0036(6)	-0.0048(6)
C28	0.0262(8)	0.0245(7)	0.0218(8)	-0.0087(6)	0.0032(6)	-0.0037(6)
C29	0.0436(10)	0.0248(8)	0.0294(9)	-0.0088(7)	0.0117(7)	-0.0087(7)
C30	0.0554(12)	0.0247(8)	0.0412(11)	-0.0140(8)	0.0127(9)	-0.0070(8)
C31	0.0472(11)	0.0340(9)	0.0363(10)	-0.0202(8)	0.0093(8)	-0.0025(8)
C32	0.0349(9)	0.0385(9)	0.0227(8)	-0.0102(7)	0.0060(7)	-0.0021(7)
C33	0.0275(8)	0.0259(8)	0.0225(8)	-0.0060(6)	0.0027(6)	-0.0016(6)
C34	0.0188(7)	0.0268(8)	0.0268(8)	-0.0091(6)	0.0017(6)	-0.0010(6)
C35	0.0232(9)	0.0337(9)	0.0688(14)	-0.0014(9)	0.0019(8)	-0.0072(7)
C36	0.0250(9)	0.0815(15)	0.0373(11)	-0.0305(10)	-0.0033(8)	0.0003(9)
C37	0.0308(9)	0.0358(9)	0.0466(11)	-0.0166(8)	-0.0052(8)	0.0089(7)
C38	0.0245(8)	0.0351(8)	0.0191(8)	-0.0096(6)	-0.0019(6)	-0.0054(6)
C39	0.0380(10)	0.0421(10)	0.0277(9)	-0.0130(7)	-0.0030(7)	-0.0121(8)
C40	0.0289(8)	0.0389(9)	0.0226(8)	-0.0060(7)	-0.0026(6)	-0.0021(7)
C41	0.0237(8)	0.0539(11)	0.0260(9)	-0.0137(8)	-0.0019(7)	-0.0029(7)
C42	0.0253(8)	0.0218(7)	0.0200(7)	-0.0049(6)	-0.0003(6)	-0.0023(6)
C43	0.0240(8)	0.0270(8)	0.0213(8)	-0.0059(6)	-0.0001(6)	-0.0054(6)
C44	0.0306(8)	0.0305(8)	0.0238(8)	-0.0069(7)	0.0021(6)	-0.0039(7)
C45	0.0303(9)	0.0435(10)	0.0253(9)	-0.0125(7)	0.0040(7)	-0.0055(7)
C46	0.0336(9)	0.0495(10)	0.0192(8)	-0.0052(7)	0.0023(7)	-0.0131(8)
C47	0.0436(10)	0.0337(9)	0.0229(8)	0.0004(7)	-0.0004(7)	-0.0133(7)
C48	0.0372(9)	0.0282(8)	0.0246(8)	-0.0064(7)	0.0008(7)	-0.0075(7)
C49	0.0485(10)	0.0197(7)	0.0162(7)	-0.0016(6)	0.0048(7)	-0.0118(7)
C50	0.0497(11)	0.0305(9)	0.0444(11)	-0.0147(8)	0.0219(9)	-0.0135(8)
C51	0.0991(19)	0.0309(10)	0.0549(14)	-0.0191(10)	0.0516(14)	-0.0213(11)
C52	0.160(3)	0.0276(10)	0.0209(10)	-0.0093(8)	0.0245(13)	-0.0373(15)
C53	0.139(3)	0.0334(11)	0.0268(10)	0.0007(9)	-0.0271(13)	-0.0352(14)
C54	0.0747(14)	0.0268(9)	0.0319(10)	-0.0009(7)	-0.0173(9)	-0.0119(9)
C55A	0.060(6)	0.052(5)	0.074(4)	-0.035(3)	-0.030(4)	0.020(3)
C56A	0.045(3)	0.066(4)	0.041(3)	-0.028(2)	-0.0022(19)	0.003(2)
C57A	0.055(3)	0.060(4)	0.049(3)	-0.007(2)	-0.021(2)	0.008(2)
C58A	0.054(3)	0.080(4)	0.039(2)	0.015(2)	-0.0145(19)	-0.005(2)
C59A	0.046(4)	0.145(10)	0.026(2)	-0.002(4)	-0.006(3)	0.022(5)
C60A	0.081(4)	0.100(6)	0.044(3)	-0.044(3)	-0.026(3)	0.044(4)

C61A	0.087(5)	0.066(3)	0.172(7)	-0.052(4)	-0.046(5)	0.003(3)
C55B	0.093(7)	0.043(4)	0.034(4)	-0.009(3)	-0.019(4)	0.003(4)
C56B	0.057(6)	0.073(7)	0.038(4)	0.016(4)	-0.007(5)	0.007(5)
C57B	0.076(6)	0.106(8)	0.039(4)	0.012(5)	-0.001(4)	0.035(6)
C58B	0.090(6)	0.067(5)	0.054(4)	-0.009(4)	-0.011(4)	0.017(4)
C59B	0.077(6)	0.057(5)	0.086(5)	-0.019(4)	-0.025(4)	0.000(4)
C60B	0.048(7)	0.064(9)	0.075(6)	-0.032(6)	-0.019(5)	0.010(5)
C61B	0.128(9)	0.063(5)	0.039(4)	-0.013(3)	-0.013(5)	-0.004(5)

6.10 Crystal structure determination of Silazine 9_{CN}

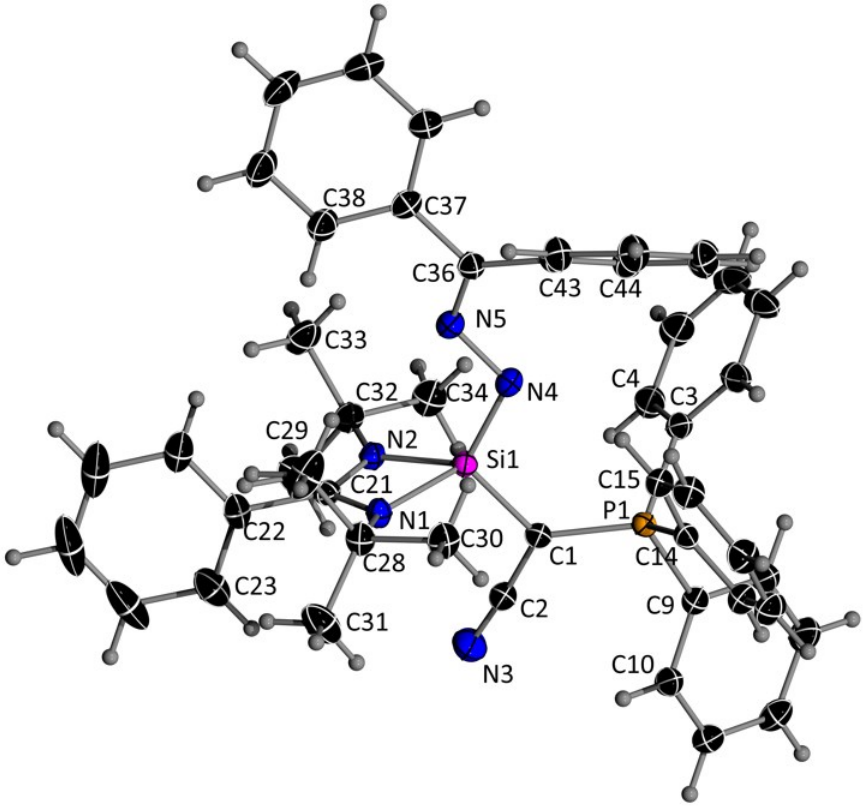


Figure S84. ORTEP of $\mathbf{9_{CN}}$. Ellipsoids are drawn at the 50% probability level.

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $\mathbf{9_{CN}}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

Atom	X	Y	Z	U(eq)
P1	0.56381(2)	0.36639(4)	0.38945(2)	0.01781(9)
Si1	0.53994(2)	0.31006(4)	0.25525(2)	0.01808(9)
N1	0.52823(6)	0.13503(12)	0.21167(5)	0.0201(2)
N2	0.59694(6)	0.31585(12)	0.20828(5)	0.0196(2)
N3	0.70028(7)	0.15201(17)	0.34300(6)	0.0376(3)
N4	0.47453(6)	0.42701(13)	0.24638(5)	0.0221(2)
N5	0.44783(6)	0.45954(13)	0.18800(5)	0.0209(2)
C4	0.60628(8)	0.65225(17)	0.37042(7)	0.0298(3)
C5	0.60357(9)	0.80928(17)	0.36767(7)	0.0362(4)
C1	0.58633(7)	0.28537(14)	0.33109(6)	0.0194(3)

C2	0.64917(7)	0.21311(15)	0.33951(6)	0.0229(3)
C3	0.55355(7)	0.57010(15)	0.38295(6)	0.0223(3)
C6	0.54783(9)	0.88387(17)	0.37651(7)	0.0372(4)
C7	0.49535(9)	0.80404(17)	0.38915(7)	0.0349(4)
C8	0.49826(8)	0.64596(16)	0.39301(6)	0.0271(3)
C9	0.62904(7)	0.33773(15)	0.45679(6)	0.0211(3)
C10	0.64464(8)	0.45467(16)	0.49787(6)	0.0273(3)
C11	0.69431(8)	0.43383(18)	0.54951(7)	0.0331(3)
C12	0.72920(8)	0.29784(18)	0.56053(6)	0.0311(3)
C13	0.71270(8)	0.18001(17)	0.52085(6)	0.0280(3)
C14	0.66254(7)	0.19910(16)	0.46928(6)	0.0245(3)
C15	0.48617(7)	0.29050(14)	0.40119(6)	0.0205(3)
C16	0.42629(7)	0.30267(16)	0.35665(6)	0.0236(3)
C17	0.36692(7)	0.23964(17)	0.36382(7)	0.0282(3)
C18	0.36706(8)	0.16292(17)	0.41477(7)	0.0294(3)
C19	0.42598(8)	0.15197(18)	0.45918(7)	0.0303(3)
C20	0.48567(7)	0.21610(16)	0.45281(6)	0.0255(3)
C21	0.57365(7)	0.18337(15)	0.18401(6)	0.0192(3)
C22	0.59593(7)	0.10217(16)	0.13751(6)	0.0247(3)
C23	0.64620(8)	-0.00738(18)	0.15356(8)	0.0352(4)
C24	0.66919(10)	-0.0812(2)	0.11058(11)	0.0533(6)
C25	0.64178(12)	-0.0460(2)	0.05251(11)	0.0605(6)
C26	0.59183(12)	0.0621(2)	0.03674(8)	0.0526(5)
C27	0.56844(9)	0.13706(19)	0.07897(7)	0.0343(4)
C28	0.47664(7)	0.01322(16)	0.19508(6)	0.0241(3)
C29	0.43172(9)	0.0400(2)	0.13356(7)	0.0433(4)
C30	0.43267(8)	0.02668(17)	0.23755(7)	0.0291(3)
C31	0.51010(9)	-0.14210(18)	0.20080(9)	0.0410(4)
C32	0.64549(7)	0.42528(16)	0.19444(6)	0.0237(3)
C33	0.61225(9)	0.50319(18)	0.13685(7)	0.0355(4)
C34	0.65896(8)	0.54283(17)	0.24298(7)	0.0323(3)
C35	0.71148(8)	0.34851(19)	0.19323(9)	0.0388(4)
C36	0.38819(7)	0.52121(15)	0.17196(6)	0.0204(3)
C37	0.36261(7)	0.55676(16)	0.10908(6)	0.0227(3)
C38	0.38740(8)	0.47806(19)	0.06778(7)	0.0309(3)
C39	0.36427(9)	0.5104(2)	0.00894(7)	0.0398(4)
C40	0.31618(9)	0.6233(2)	-0.01049(7)	0.0388(4)
C41	0.29191(8)	0.70361(18)	0.02981(7)	0.0332(3)
C42	0.31433(7)	0.67026(16)	0.08890(6)	0.0264(3)
C43	0.34429(7)	0.54889(15)	0.21182(6)	0.0209(3)
C44	0.27917(7)	0.48833(17)	0.19834(6)	0.0260(3)
C45	0.23816(7)	0.50427(18)	0.23604(7)	0.0303(3)
C46	0.26159(8)	0.58198(18)	0.28779(7)	0.0296(3)
C47	0.32628(8)	0.64346(17)	0.30188(6)	0.0283(3)
C48	0.36762(7)	0.62673(15)	0.26437(6)	0.0238(3)

Table S23. Anisotropic displacement parameters(Å^2) for **9$_{CN}$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2 h k a^* b^* U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P1	0.02107(17)	0.01520(16)	0.01680(16)	-0.00034(12)	0.00437(13)	0.00016(12)
Si1	0.01945(18)	0.01830(18)	0.01680(18)	-0.00055(13)	0.00533(14)	-0.00032(13)
N1	0.0212(5)	0.0206(6)	0.0197(6)	-0.0017(4)	0.0074(4)	-0.0025(4)
N2	0.0213(6)	0.0193(5)	0.0193(5)	0.0003(4)	0.0074(4)	-0.0022(4)
N3	0.0334(7)	0.0453(8)	0.0346(7)	0.0019(6)	0.0099(6)	0.0152(6)
N4	0.0242(6)	0.0236(6)	0.0180(5)	0.0006(4)	0.0044(4)	0.0009(5)
N5	0.0220(6)	0.0216(5)	0.0186(5)	0.0009(4)	0.0046(4)	-0.0016(4)
C4	0.0406(9)	0.0226(7)	0.0276(7)	-0.0017(6)	0.0112(6)	-0.0046(6)
C5	0.0552(10)	0.0236(8)	0.0297(8)	-0.0007(6)	0.0109(7)	-0.0098(7)
C1	0.0211(6)	0.0182(6)	0.0191(6)	0.0001(5)	0.0054(5)	0.0004(5)
C2	0.0262(7)	0.0231(7)	0.0195(7)	0.0007(5)	0.0063(5)	0.0010(6)
C3	0.0304(7)	0.0173(6)	0.0169(6)	-0.0014(5)	0.0022(5)	-0.0002(5)
C6	0.0591(11)	0.0169(7)	0.0266(8)	-0.0012(6)	-0.0045(7)	-0.0011(7)
C7	0.0411(9)	0.0238(7)	0.0314(8)	-0.0082(6)	-0.0053(7)	0.0084(7)
C8	0.0302(8)	0.0234(7)	0.0237(7)	-0.0040(6)	0.0001(6)	0.0029(6)
C9	0.0231(7)	0.0220(6)	0.0183(6)	-0.0002(5)	0.0056(5)	-0.0023(5)
C10	0.0359(8)	0.0215(7)	0.0227(7)	-0.0018(6)	0.0046(6)	0.0015(6)
C11	0.0450(9)	0.0290(8)	0.0211(7)	-0.0044(6)	0.0013(6)	-0.0032(7)
C12	0.0325(8)	0.0368(8)	0.0203(7)	0.0035(6)	0.0005(6)	-0.0016(6)
C13	0.0304(8)	0.0293(7)	0.0236(7)	0.0047(6)	0.0055(6)	0.0039(6)
C14	0.0289(7)	0.0218(7)	0.0218(7)	-0.0002(5)	0.0053(6)	0.0001(6)
C15	0.0247(7)	0.0168(6)	0.0214(7)	-0.0023(5)	0.0085(5)	0.0010(5)
C16	0.0257(7)	0.0241(7)	0.0217(7)	0.0004(5)	0.0076(6)	0.0006(6)
C17	0.0238(7)	0.0324(8)	0.0283(8)	-0.0004(6)	0.0065(6)	-0.0001(6)
C18	0.0262(7)	0.0308(8)	0.0349(8)	0.0012(6)	0.0144(6)	-0.0031(6)
C19	0.0331(8)	0.0331(8)	0.0278(8)	0.0064(6)	0.0136(6)	0.0001(6)
C20	0.0275(7)	0.0268(7)	0.0229(7)	0.0018(6)	0.0078(6)	0.0003(6)
C21	0.0186(6)	0.0202(6)	0.0180(6)	0.0019(5)	0.0034(5)	0.0015(5)
C22	0.0263(7)	0.0229(7)	0.0288(7)	-0.0057(6)	0.0143(6)	-0.0067(6)
C23	0.0319(8)	0.0268(8)	0.0520(10)	-0.0045(7)	0.0202(7)	-0.0024(6)
C24	0.0499(11)	0.0298(9)	0.0965(17)	-0.0188(10)	0.0484(11)	-0.0057(8)
C25	0.0787(15)	0.0519(12)	0.0729(15)	-0.0324(11)	0.0589(13)	-0.0234(11)
C26	0.0730(13)	0.0577(12)	0.0377(10)	-0.0208(9)	0.0331(10)	-0.0257(11)
C27	0.0430(9)	0.0369(9)	0.0265(8)	-0.0071(6)	0.0153(7)	-0.0115(7)
C28	0.0257(7)	0.0228(7)	0.0254(7)	-0.0041(5)	0.0095(6)	-0.0078(6)
C29	0.0391(9)	0.0607(11)	0.0276(8)	-0.0037(8)	0.0045(7)	-0.0244(8)
C30	0.0281(7)	0.0299(8)	0.0325(8)	-0.0017(6)	0.0137(6)	-0.0071(6)
C31	0.0447(10)	0.0228(8)	0.0648(12)	-0.0052(7)	0.0309(9)	-0.0059(7)
C32	0.0257(7)	0.0220(7)	0.0257(7)	0.0025(6)	0.0105(6)	-0.0055(6)
C33	0.0508(10)	0.0283(8)	0.0274(8)	0.0058(6)	0.0103(7)	-0.0084(7)
C34	0.0376(8)	0.0282(8)	0.0319(8)	-0.0032(6)	0.0106(7)	-0.0132(6)
C35	0.0282(8)	0.0335(8)	0.0598(11)	0.0000(8)	0.0205(8)	-0.0049(7)
C36	0.0207(6)	0.0203(6)	0.0208(7)	0.0003(5)	0.0065(5)	-0.0011(5)
C37	0.0205(6)	0.0251(7)	0.0223(7)	0.0033(5)	0.0053(5)	-0.0040(5)

C38	0.0299(8)	0.0393(8)	0.0255(8)	0.0053(6)	0.0109(6)	0.0059(7)
C39	0.0420(9)	0.0562(11)	0.0255(8)	0.0078(7)	0.0167(7)	0.0072(8)
C40	0.0383(9)	0.0546(11)	0.0243(8)	0.0146(7)	0.0095(7)	0.0004(8)
C41	0.0298(8)	0.0343(8)	0.0336(8)	0.0137(7)	0.0050(6)	0.0012(6)
C42	0.0244(7)	0.0254(7)	0.0288(8)	0.0029(6)	0.0058(6)	-0.0026(6)
C43	0.0220(6)	0.0191(6)	0.0219(7)	0.0022(5)	0.0063(5)	0.0028(5)
C44	0.0247(7)	0.0286(7)	0.0251(7)	-0.0051(6)	0.0071(6)	-0.0013(6)
C45	0.0248(7)	0.0350(8)	0.0330(8)	-0.0030(6)	0.0110(6)	-0.0024(6)
C46	0.0295(7)	0.0351(8)	0.0277(8)	-0.0016(6)	0.0135(6)	0.0053(6)
C47	0.0312(8)	0.0296(8)	0.0241(7)	-0.0045(6)	0.0071(6)	0.0044(6)
C48	0.0234(7)	0.0226(7)	0.0247(7)	-0.0009(5)	0.0050(6)	0.0011(5)

6.11 Crystal structure determination of 10

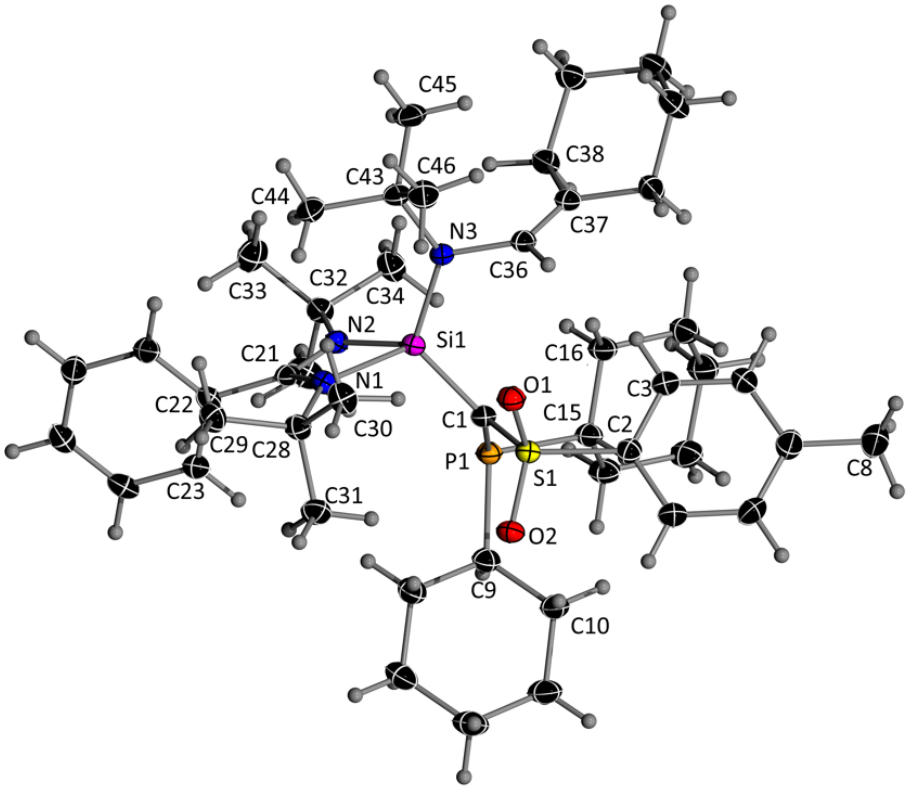


Figure S85. ORTEP of **10**. Ellipsoids are drawn at the 50% probability level.

Table S24. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **10**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor for all atoms.

Atom	X	Y	Z	U(eq)
S1	0.23568(3)	0.66812(2)	0.19612(2)	0.01822(9)
P1	0.42169(3)	0.58382(2)	0.21623(2)	0.01960(9)
Si1	0.42574(3)	0.66932(2)	0.36008(2)	0.01628(9)
O1	0.20710(9)	0.70555(3)	0.26089(7)	0.0227(2)
N1	0.51412(10)	0.72414(4)	0.33722(8)	0.0180(2)
C1	0.35322(12)	0.63697(5)	0.25617(9)	0.0184(3)
O2	0.25105(8)	0.68600(4)	0.10397(6)	0.0222(2)
N2	0.58335(10)	0.65437(4)	0.38925(8)	0.0182(2)

N3	0.36137(10)	0.67170(4)	0.45902(8)	0.0183(2)
C2	0.10674(12)	0.63033(5)	0.16968(9)	0.0202(3)
C3	0.06984(12)	0.60450(5)	0.24192(10)	0.0226(3)
C4	-0.03292(13)	0.57697(5)	0.22345(10)	0.0228(3)
C5	-0.10197(13)	0.57466(5)	0.13318(11)	0.0270(3)
C6	-0.06516(14)	0.60155(6)	0.06199(11)	0.0331(4)
C7	0.03860(13)	0.62908(6)	0.07931(10)	0.0268(3)
C8	-0.21240(15)	0.54355(7)	0.11417(12)	0.0381(4)
C9	0.31060(13)	0.53386(5)	0.21195(9)	0.0218(3)
C10	0.29129(13)	0.52287(5)	0.31251(10)	0.0241(3)
C11	0.19820(14)	0.48328(5)	0.31279(10)	0.0272(3)
C12	0.23394(15)	0.43675(5)	0.26744(11)	0.0300(3)
C13	0.25883(15)	0.44685(5)	0.16857(11)	0.0299(3)
C14	0.35157(14)	0.48697(5)	0.16960(10)	0.0261(3)
C15	0.43314(13)	0.58798(5)	0.08870(10)	0.0233(3)
C16	0.32058(13)	0.58506(5)	0.01150(10)	0.0247(3)
C17	0.35422(15)	0.58031(6)	-0.08632(10)	0.0311(3)
C18	0.43138(16)	0.62287(6)	-0.10601(11)	0.0339(4)
C19	0.54150(14)	0.62842(6)	-0.02807(11)	0.0308(3)
C20	0.50846(13)	0.63170(5)	0.07036(10)	0.0262(3)
C21	0.61375(12)	0.69803(5)	0.36007(9)	0.0183(3)
C22	0.73798(12)	0.71241(5)	0.35536(9)	0.0194(3)
C23	0.78793(13)	0.69716(5)	0.27916(10)	0.0220(3)
C24	0.90656(13)	0.70730(5)	0.27777(10)	0.0245(3)
C25	0.97505(13)	0.73261(5)	0.35153(11)	0.0254(3)
C26	0.92497(13)	0.74793(5)	0.42709(10)	0.0249(3)
C27	0.80637(12)	0.73821(5)	0.42952(10)	0.0220(3)
C28	0.49868(12)	0.77171(5)	0.28568(10)	0.0211(3)
C29	0.38375(13)	0.79489(5)	0.30440(11)	0.0268(3)
C30	0.48982(14)	0.76232(5)	0.17979(10)	0.0270(3)
C31	0.60124(13)	0.80710(5)	0.32006(11)	0.0255(3)
C32	0.66283(12)	0.61499(5)	0.43692(10)	0.0212(3)
C33	0.75082(14)	0.63437(6)	0.52203(11)	0.0320(3)
C34	0.73056(14)	0.59005(6)	0.36827(12)	0.0317(3)
C35	0.58119(13)	0.57829(5)	0.47133(11)	0.0280(3)
C36	0.24439(12)	0.64993(5)	0.45161(9)	0.0195(3)
C37	0.21706(12)	0.60874(5)	0.49180(9)	0.0208(3)
C38	0.30165(13)	0.57313(5)	0.54868(10)	0.0234(3)
C39	0.26582(13)	0.55946(6)	0.64319(10)	0.0273(3)
C40	0.13594(14)	0.54376(6)	0.62983(11)	0.0302(3)
C41	0.05430(14)	0.58242(6)	0.57695(11)	0.0308(3)
C42	0.08783(12)	0.59370(6)	0.48095(10)	0.0253(3)
C43	0.38507(12)	0.70777(5)	0.54063(9)	0.0214(3)
C44	0.28485(14)	0.74562(6)	0.52815(11)	0.0279(3)
C45	0.50453(13)	0.73351(5)	0.54675(10)	0.0253(3)
C46	0.38922(15)	0.68078(6)	0.63430(10)	0.0297(3)

Table S25. Anisotropic displacement parameters(Å^2) for **9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2\ h\ k\ a^*\ b^*\ U^{12}]$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	0.01967(16)	0.01988(16)	0.01530(16)	0.00062(12)	0.00377(12)	-0.00120(12)
P1	0.02307(18)	0.02075(18)	0.01570(17)	-0.00115(12)	0.00545(13)	-0.00038(13)
Si1	0.01720(18)	0.01772(18)	0.01446(17)	0.00012(13)	0.00434(13)	-0.00009(13)
O1	0.0270(5)	0.0222(5)	0.0198(5)	-0.0016(4)	0.0065(4)	-0.0003(4)
N1	0.0190(5)	0.0182(5)	0.0174(5)	0.0010(4)	0.0052(4)	-0.0001(4)
C1	0.0201(6)	0.0205(6)	0.0148(6)	-0.0006(5)	0.0040(5)	-0.0007(5)
O2	0.0250(5)	0.0253(5)	0.0170(5)	0.0039(4)	0.0055(4)	-0.0010(4)
N2	0.0176(5)	0.0197(6)	0.0177(5)	0.0012(4)	0.0042(4)	0.0006(4)
N3	0.0190(5)	0.0215(6)	0.0150(5)	-0.0021(4)	0.0045(4)	-0.0025(4)
C2	0.0195(6)	0.0212(7)	0.0199(7)	-0.0012(5)	0.0037(5)	0.0003(5)
C3	0.0240(7)	0.0255(7)	0.0179(7)	0.0001(5)	0.0032(5)	-0.0006(6)
C4	0.0239(7)	0.0226(7)	0.0230(7)	0.0012(5)	0.0074(6)	-0.0008(6)
C5	0.0251(7)	0.0271(7)	0.0277(7)	-0.0018(6)	0.0021(6)	-0.0032(6)
C6	0.0331(8)	0.0418(9)	0.0210(7)	0.0007(6)	-0.0038(6)	-0.0087(7)
C7	0.0292(8)	0.0319(8)	0.0189(7)	0.0028(6)	0.0032(6)	-0.0040(6)
C8	0.0344(9)	0.0430(10)	0.0341(9)	0.0005(7)	-0.0005(7)	-0.0132(7)
C9	0.0277(7)	0.0212(7)	0.0174(6)	-0.0006(5)	0.0069(5)	-0.0016(6)
C10	0.0323(8)	0.0229(7)	0.0182(7)	-0.0011(5)	0.0075(6)	-0.0023(6)
C11	0.0344(8)	0.0251(7)	0.0238(7)	0.0003(6)	0.0098(6)	-0.0037(6)
C12	0.0409(9)	0.0231(7)	0.0272(8)	-0.0005(6)	0.0092(7)	-0.0056(6)
C13	0.0424(9)	0.0236(7)	0.0248(7)	-0.0052(6)	0.0093(7)	-0.0038(6)
C14	0.0350(8)	0.0235(7)	0.0213(7)	-0.0028(6)	0.0090(6)	-0.0001(6)
C15	0.0265(7)	0.0256(7)	0.0195(7)	-0.0021(5)	0.0086(6)	-0.0010(6)
C16	0.0304(8)	0.0269(7)	0.0175(7)	-0.0018(5)	0.0063(6)	-0.0027(6)
C17	0.0442(9)	0.0323(8)	0.0180(7)	-0.0024(6)	0.0086(6)	-0.0031(7)
C18	0.0485(10)	0.0345(9)	0.0218(7)	0.0011(6)	0.0140(7)	-0.0032(7)
C19	0.0362(8)	0.0313(8)	0.0293(8)	0.0015(6)	0.0178(7)	-0.0020(7)
C20	0.0284(8)	0.0275(8)	0.0247(7)	-0.0016(6)	0.0102(6)	-0.0022(6)
C21	0.0214(7)	0.0206(7)	0.0135(6)	-0.0019(5)	0.0049(5)	0.0000(5)
C22	0.0198(7)	0.0193(6)	0.0196(6)	0.0030(5)	0.0055(5)	0.0009(5)
C23	0.0260(7)	0.0218(7)	0.0189(7)	0.0009(5)	0.0062(5)	0.0002(5)
C24	0.0264(7)	0.0260(7)	0.0240(7)	0.0064(6)	0.0123(6)	0.0047(6)
C25	0.0196(7)	0.0268(7)	0.0306(8)	0.0090(6)	0.0065(6)	0.0015(6)
C26	0.0230(7)	0.0245(7)	0.0257(7)	0.0028(6)	0.0007(6)	-0.0031(6)
C27	0.0242(7)	0.0225(7)	0.0199(7)	0.0002(5)	0.0056(5)	-0.0003(5)
C28	0.0244(7)	0.0179(6)	0.0212(7)	0.0027(5)	0.0045(5)	-0.0001(5)
C29	0.0264(7)	0.0204(7)	0.0341(8)	0.0034(6)	0.0069(6)	0.0024(6)
C30	0.0336(8)	0.0258(7)	0.0213(7)	0.0047(6)	0.0042(6)	-0.0032(6)
C31	0.0279(7)	0.0207(7)	0.0281(7)	0.0018(6)	0.0055(6)	-0.0027(6)
C32	0.0194(7)	0.0215(7)	0.0228(7)	0.0046(5)	0.0040(5)	0.0031(5)
C33	0.0306(8)	0.0291(8)	0.0318(8)	0.0056(6)	-0.0054(6)	0.0013(6)
C34	0.0322(8)	0.0293(8)	0.0366(9)	0.0064(7)	0.0146(7)	0.0112(6)
C35	0.0234(7)	0.0273(8)	0.0328(8)	0.0106(6)	0.0039(6)	0.0011(6)
C36	0.0189(6)	0.0250(7)	0.0149(6)	-0.0012(5)	0.0042(5)	0.0005(5)

C37	0.0219(7)	0.0258(7)	0.0155(6)	-0.0017(5)	0.0060(5)	-0.0001(5)
C38	0.0235(7)	0.0258(7)	0.0221(7)	0.0024(6)	0.0075(6)	0.0008(6)
C39	0.0299(8)	0.0304(8)	0.0222(7)	0.0066(6)	0.0063(6)	0.0001(6)
C40	0.0317(8)	0.0316(8)	0.0297(8)	0.0100(6)	0.0121(6)	0.0002(6)
C41	0.0261(8)	0.0360(9)	0.0337(8)	0.0097(7)	0.0139(6)	0.0018(6)
C42	0.0216(7)	0.0305(8)	0.0242(7)	0.0048(6)	0.0055(6)	-0.0025(6)
C43	0.0253(7)	0.0240(7)	0.0160(6)	-0.0042(5)	0.0062(5)	-0.0013(6)
C44	0.0296(8)	0.0278(8)	0.0276(8)	-0.0061(6)	0.0090(6)	0.0011(6)
C45	0.0265(7)	0.0288(8)	0.0209(7)	-0.0072(6)	0.0052(6)	-0.0038(6)
C46	0.0423(9)	0.0306(8)	0.0165(7)	-0.0040(6)	0.0063(6)	-0.0060(7)

7 Computational Details

7.1 General remarks

All calculations were performed without symmetry restrictions. Starting coordinates were obtained with GaussView 6.0[40] or directly from the crystal structure analyses if accessible. The geometry optimizations were carried out with the Gaussian16 (Revision C.01)[41] program package. The geometry optimizations were performed using Density Functional Theory (DFT)[31] with the PBE0[32] functional using the def2svp[42] in conjunction with Grimme's D3 dispersion correction[43] with Becke-Johnson damping[44]. Harmonic vibrational frequency analyses were performed at the same level of theory as the optimizations to determine the nature of the structure. The vibrational frequency analysis showed no imaginary frequencies. Single point energies were calculated using the def2tzvpp[42] basis set. The NBO analysis was performed with NBO Version 7.0[45] using the def2tzvpp basis set. The optimized structures were used for the quantum theory of atoms in molecules (QTAIM)[46] and noncovalent interaction (NCI)[47] analyses using Multiwfn[48] to depict the topological properties of the molecules. The results were visualized using the VMD 1.9.4a51 software.[49]

7.2 Hydrogen Bonding in Silanone 6

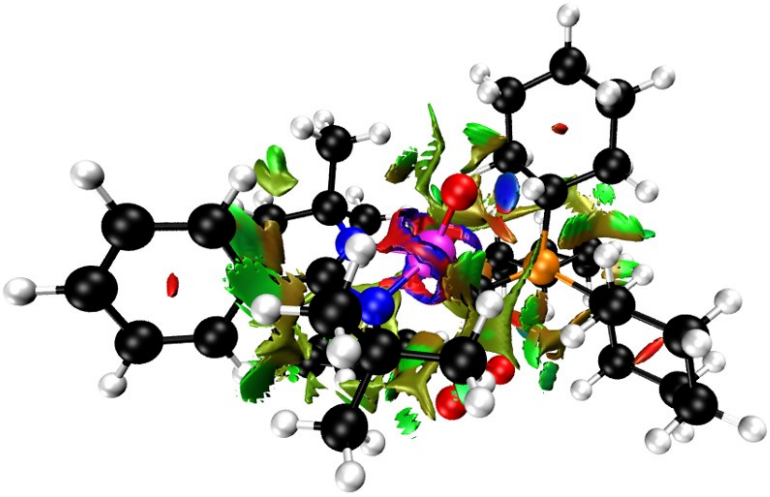


Figure S86. NCI plot for the silanone **6** coloured in a blue-green-red scheme over the range of -0.035 < sign(λ2)ρ < 0.02 and isosurface of RDG = 0.3. Blue indicates strong attraction, green indicates weak interaction, and red indicates repulsion.

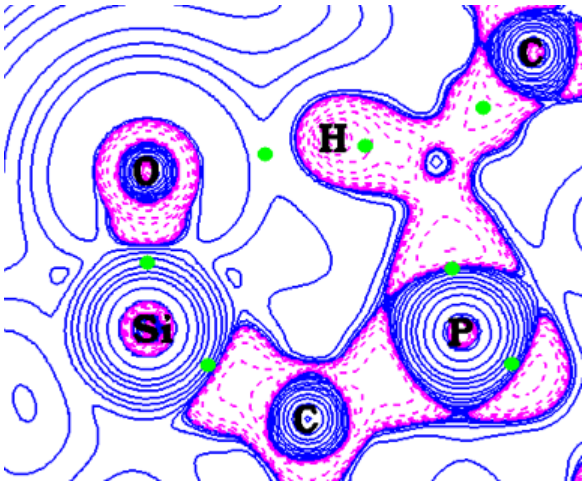
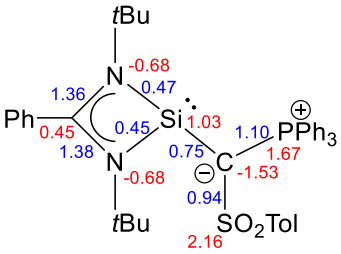
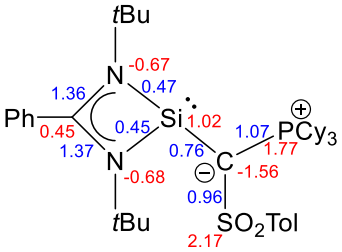


Figure S87. Contour plot of the Laplacian of the electron density around the Si-O bond in silanone 6 to showcase the bond critical point (BCP) between the oxygen atom and the hydrogen atom. Electron density ρ(r) = 0.035 au, Laplacian of the electron density $\nabla^2\rho(r)$ = 0.111 au, Kinetic energy density G(r) = 0.027 au, Potential energy density V(r) = -0.026, Total electronic energy density H(r) = 0.0006 au, and bond ellipticity $\varepsilon(r_c)$ = 0.047.

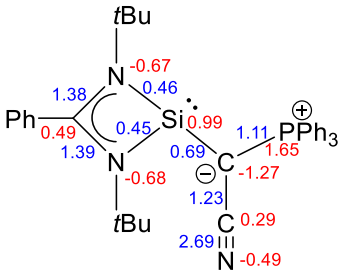
7.3 Results of the NBO analysis



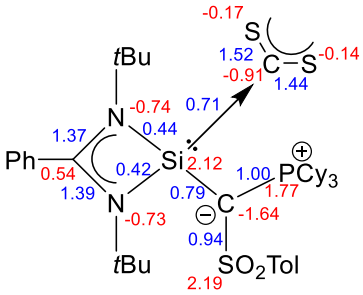
AYSi-1



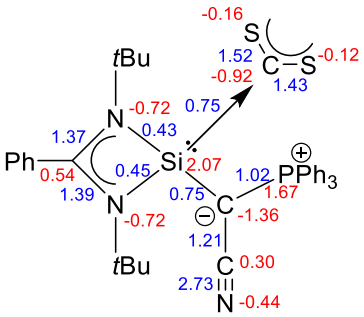
AYSi-2



AYSi-3

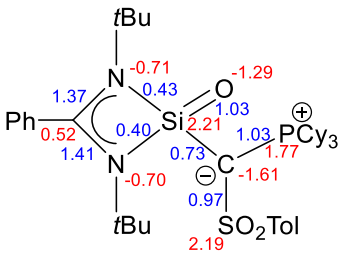


5_{Ts}

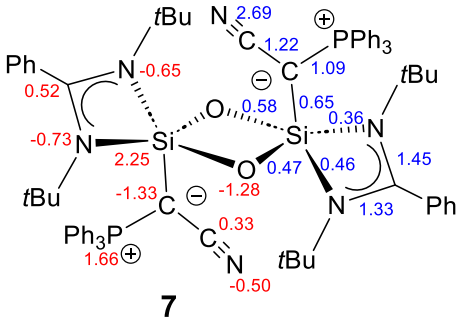


5_{CN}

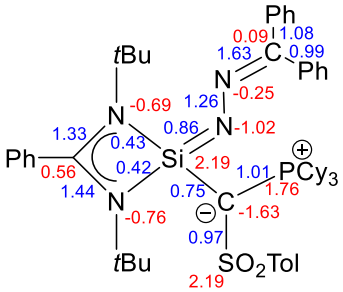
Wiberg Bond Index
NPA Charge



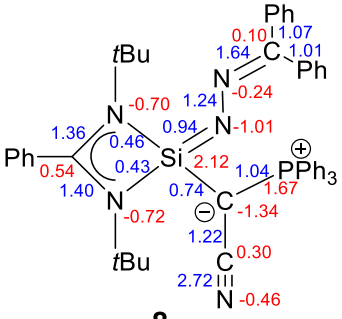
6



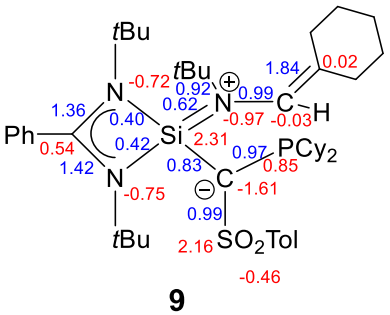
7



8_{Ts}



8_{CN}



9

Figure S88. Wiberg Bond Indeces (blue) and NPA charges (red) for **AYSi-1**, **AYSI-2**, **AYSi-3**, **4-9** calculated at the PBE0/def2tzvpp level of theory.

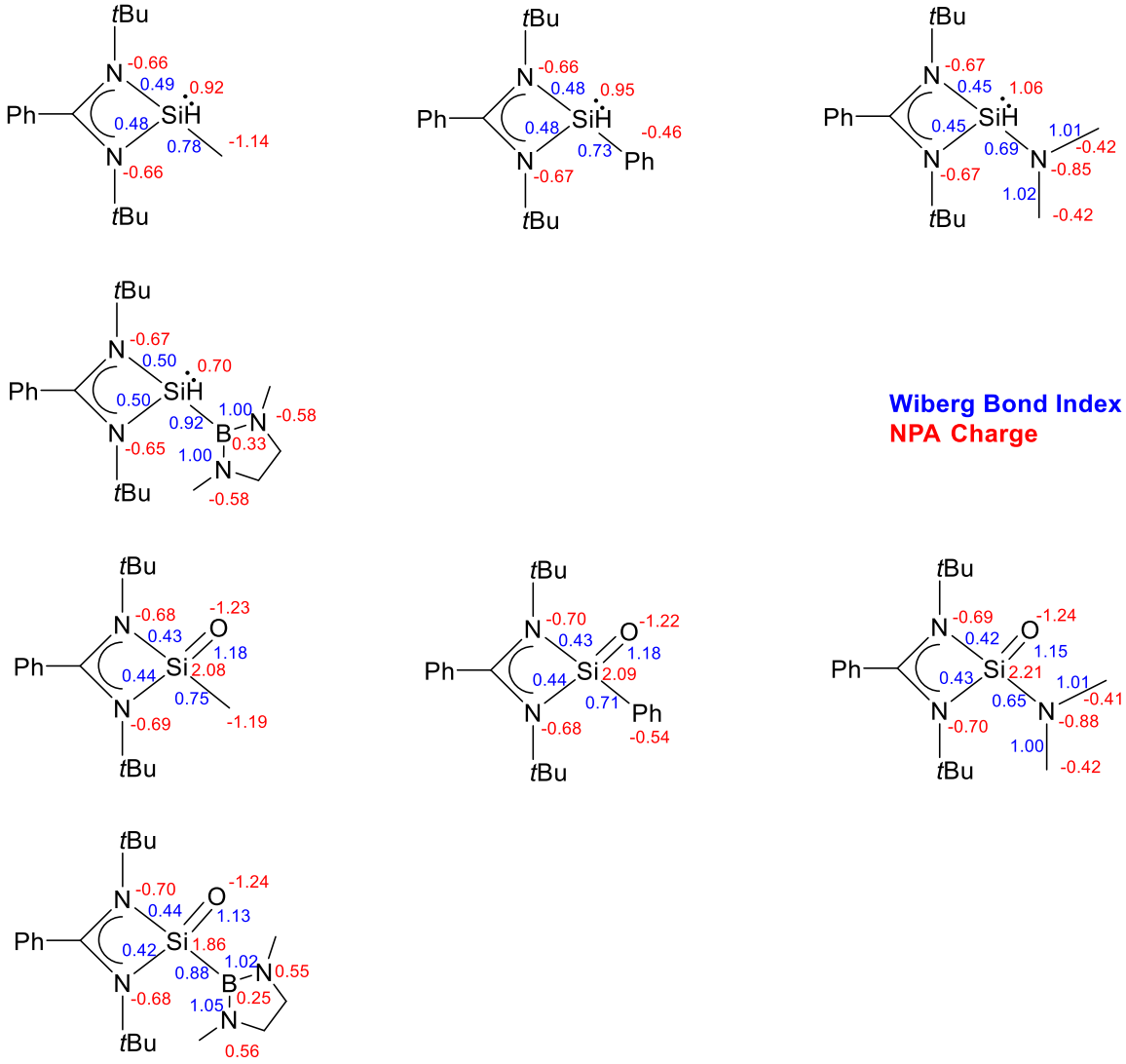


Figure S89. Wiberg Bond Indeces (blue) and NPA charges (red) for amidine-substituted silylenes and their respective silanones calculated at the PBE0/def2tzvpp level of theory.

Table S26. Second order perturbation theory analysis of Fock Matrix in NBO Basis of Silanone 6

Donor (L) NBO	Acceptor (NL) NBO	*E*(2) (kcal/mol)	E(NL)-E(L) (a.u.)	F(L,NL) (a.u.)
from unit 3 to unit 1				
LP (1) O112	BD*(1) C 9- H 19	2.99	0.90	0.046
LP (2) O112	BD*(1) C 9- H 19	6.76	0.64	0.059
LP (3) O112	BD*(1) C 9- H 19	2.47	0.64	0.035

Table S27. Second order perturbation theory analysis of Fock Matrix in NBO Basis of AYSi-2

Donor (L) NBO	Acceptor (NL) NBO	*E*(2) (kcal/mol)	E(NL)-E(L) (a.u.)	F(L,NL) (a.u.)
within unit 1				
BD (1) C 3-Si 7	BD*(1) S 1- O 2	2.97	0.74	0.042

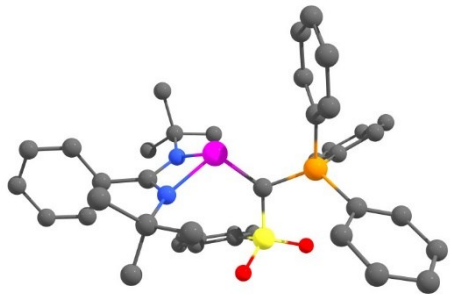
Table S28. NBO analysis of different amidine-substituted silylenes with substituents R.

R	WBI Si-R	HOMO (kcal/mol)	LUMO (kcal/mol)	DE_{H-L} (kcal/mol)
Me	0.78	-115.59	-20.77	94.82
Ph	0.73	-120.62	-22.98	97.64
NMe_2	0.69	-121.53	-20.19	101.34
BR_2	0.92	-108.07	-20.44	87.63
PhYCN (AYSi-3)	0.69	-115.17	-28.24	86.93
CyYTos (AYSi-2)	0.76	-111.33	-17.16	93.73
Bis(amidinato)	0.95 (avg.)	-100.41	-21.08	79.33

Table S29. NBO analysis of different amidine-substituted silylanones with substituents R.

R	WBI Si-R	WBI Si-O	DE_{H-L} (kcal/mol)
Me	0.75	1.18	119.45
Ph	0.71	1.18	121.53
NMe_2	0.65	1.15	109.07
BR_2	0.88	1.13	100.77
PhYCN (AYSi-3)	0.68	1.09	101.46
CyYTos (AYSi-2)	0.73	1.03	113.22

7.4 Coordinates of the optimized structures

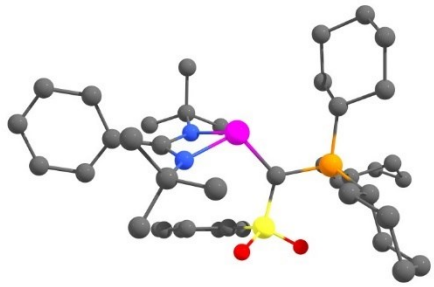


AYSi-1

E = -2876.71922576

S	2.181465000	3.900648000	5.849055000
O	0.842128000	4.511608000	5.673936000
C	3.252165000	4.710083000	4.765808000
O	2.294353000	2.436468000	5.745766000
C	2.642168000	4.265856000	7.540428000
Si	5.099748000	4.500473000	4.505359000
C	1.959448000	5.262434000	8.231882000
C	3.606225000	3.493870000	8.182182000
N	5.551244000	2.827561000	5.273516000
N	5.935469000	4.707522000	6.213249000
C	6.273790000	3.419115000	6.229056000
H	1.148866000	5.795281000	7.731681000
C	2.296456000	5.531211000	9.556779000
C	3.922076000	3.762301000	9.508615000
H	4.081307000	2.679318000	7.633875000
C	5.564987000	1.458248000	4.759326000
C	6.462779000	5.878005000	6.907364000
C	7.379955000	2.810893000	7.014049000
H	1.762276000	6.316123000	10.099201000
C	3.289526000	4.796377000	10.213202000
H	4.675539000	3.155534000	10.019172000
C	4.569753000	1.435054000	3.598463000
C	5.080008000	0.484819000	5.836383000
C	6.953562000	1.061738000	4.249854000
C	5.317394000	6.893070000	6.935082000
C	6.888781000	5.574429000	8.344090000
C	7.643594000	6.463391000	6.123876000
C	7.136121000	2.105637000	8.195679000
C	8.698614000	2.966793000	6.570293000
C	3.678458000	5.100798000	11.629645000
H	4.872083000	2.150211000	2.815928000
H	3.572714000	1.704784000	3.974763000
H	4.528331000	0.430469000	3.152425000
H	5.011972000	-0.532593000	5.421431000
H	4.080929000	0.786901000	6.182874000
H	5.774077000	0.449776000	6.688034000
H	6.907629000	0.080082000	3.753641000
H	7.685007000	0.990094000	5.066909000
H	7.315669000	1.801659000	3.519347000
H	4.959610000	7.098296000	5.914388000
H	5.648187000	7.841299000	7.384627000
H	4.471168000	6.498614000	7.516008000
H	7.783143000	4.939384000	8.391273000
H	6.074939000	5.078641000	8.891045000

H	7.121697000	6.519960000	8.857003000
H	7.347248000	6.665603000	5.083756000
H	8.490437000	5.761768000	6.109709000
H	7.988341000	7.402049000	6.585398000
H	6.111095000	1.980901000	8.547650000
C	8.194632000	1.572752000	8.928377000
C	9.755440000	2.432619000	7.302321000
H	8.889568000	3.503261000	5.638163000
H	4.663182000	5.595972000	11.666089000
H	3.756311000	4.182649000	12.231460000
H	2.952485000	5.767892000	12.114888000
H	7.992602000	1.026138000	9.852403000
C	9.505800000	1.737184000	8.485427000
H	10.780538000	2.558032000	6.945848000
H	10.335168000	1.319798000	9.061135000
P	2.354498000	5.623498000	3.604803000
C	3.476208000	6.129908000	2.262380000
C	3.568963000	5.403831000	1.072956000
C	4.301651000	7.244105000	2.461438000
C	4.489385000	5.781673000	0.096871000
H	2.922298000	4.540787000	0.905077000
C	5.216243000	7.619115000	1.483642000
H	4.226896000	7.819979000	3.386866000
C	5.314654000	6.884896000	0.301738000
H	4.558432000	5.208916000	-0.830739000
H	5.860665000	8.485653000	1.647811000
H	6.035914000	7.177795000	-0.465014000
C	1.692625000	7.224201000	4.170139000
C	1.146378000	8.142311000	3.264083000
C	1.836884000	7.577918000	5.511360000
C	0.713083000	9.387695000	3.711771000
H	1.079846000	7.894314000	2.201586000
C	1.408341000	8.826816000	5.955954000
H	2.309499000	6.873265000	6.195585000
C	0.838017000	9.728530000	5.059263000
H	0.285706000	10.100799000	3.002964000
H	1.526581000	9.096324000	7.008127000
H	0.501437000	10.708125000	5.407246000
C	1.011023000	4.684359000	2.811514000
C	-0.248396000	5.221011000	2.535372000
C	1.281196000	3.347671000	2.495739000
C	-1.218982000	4.433699000	1.920453000
H	-0.488301000	6.244313000	2.826750000
C	0.309098000	2.567189000	1.876640000
H	2.246026000	2.913345000	2.766080000
C	-0.940801000	3.110151000	1.583231000
H	-2.205666000	4.855686000	1.715655000
H	0.525973000	1.523233000	1.639372000
H	-1.707110000	2.494493000	1.106222000



AYSi-2

E = -2887.60483548

S	2.163801000	4.091619000	5.787871000
O	0.826602000	4.718032000	5.630017000
C	3.249970000	4.813451000	4.674153000
O	2.211975000	2.619388000	5.737678000
C	2.649513000	4.503722000	7.460681000
P	2.451801000	5.740004000	3.420843000
Si	5.073723000	4.411116000	4.502157000
C	2.089067000	5.618124000	8.078989000
C	3.511174000	3.666713000	8.162585000
C	3.790996000	6.342023000	2.292083000
C	1.443921000	7.147177000	4.051065000
C	1.321098000	4.784505000	2.304837000
N	5.422839000	2.746045000	5.329058000
N	5.923179000	4.633756000	6.203604000
C	6.178082000	3.327943000	6.264960000
H	1.356823000	6.217949000	7.537101000
C	2.447311000	5.929198000	9.388080000
C	3.850658000	3.980929000	9.473787000
H	3.888236000	2.768451000	7.671964000
H	4.480475000	5.473647000	2.285990000
C	4.590757000	7.500726000	2.892286000
C	3.403207000	6.640816000	0.841482000
H	0.595711000	6.608906000	4.505197000
C	2.111359000	7.930020000	5.181644000
C	0.905264000	8.085039000	2.970784000
H	1.246219000	5.415916000	1.401818000
C	-0.107684000	4.537605000	2.794003000
C	2.002403000	3.467303000	1.928386000
C	5.365211000	1.354560000	4.875060000
C	6.532598000	5.783816000	6.867947000
C	7.240868000	2.678383000	7.075495000
H	2.010627000	6.807785000	9.870638000
C	3.342515000	5.125412000	10.103113000
H	4.523068000	3.322436000	10.031353000
H	3.964796000	8.408172000	2.931546000
H	4.877038000	7.260747000	3.926890000
C	5.836794000	7.781826000	2.062882000
C	4.648302000	6.953746000	0.012581000
H	2.885704000	5.783547000	0.387601000
H	2.704777000	7.494142000	0.795663000
H	2.512050000	7.233822000	5.930836000
H	2.971711000	8.500602000	4.798051000
C	1.110896000	8.897509000	5.802823000
C	-0.084503000	9.072824000	3.585753000
H	1.737305000	8.644359000	2.508800000
H	0.416747000	7.520721000	2.160378000
H	-0.083314000	3.969385000	3.734224000

H	-0.605980000	5.490589000	3.031039000
C	-0.906205000	3.783892000	1.734590000
C	1.196892000	2.696753000	0.889319000
H	3.029992000	3.641120000	1.567588000
H	2.104006000	2.868481000	2.846888000
C	4.407524000	1.336571000	3.685488000
C	4.787541000	0.465286000	5.979000000
C	6.738829000	0.845689000	4.428426000
C	5.442631000	6.854020000	6.951434000
C	7.012948000	5.473263000	8.286698000
C	7.701294000	6.307442000	6.024858000
C	6.948227000	2.030284000	8.278105000
C	8.568281000	2.737672000	6.634552000
C	3.760583000	5.476539000	11.500318000
H	6.399553000	8.619747000	2.505294000
H	6.495560000	6.896478000	2.112356000
C	5.477327000	8.081466000	0.613590000
H	5.269367000	6.042372000	-0.048165000
H	4.351925000	7.198131000	-1.020365000
H	0.293155000	8.319695000	6.270485000
H	1.591540000	9.472090000	6.611265000
C	0.529791000	9.839779000	4.752689000
H	-0.448179000	9.771875000	2.815180000
H	-0.967817000	8.513375000	3.942159000
H	-1.927988000	3.601372000	2.104572000
H	-1.010311000	4.412492000	0.830367000
C	-0.235147000	2.468461000	1.357306000
H	1.186749000	3.261722000	-0.061228000
H	1.692239000	1.736047000	0.674649000
H	4.780159000	1.986330000	2.877586000
H	3.421593000	1.694109000	4.010802000
H	4.310119000	0.314566000	3.290810000
H	4.666237000	-0.563936000	5.607666000
H	3.801051000	0.846690000	6.279657000
H	5.453010000	0.425776000	6.852941000
H	6.636978000	-0.147139000	3.963992000
H	7.438321000	0.750623000	5.270209000
H	7.175606000	1.530424000	3.685002000
H	5.023591000	7.059494000	5.956431000
H	5.850743000	7.791455000	7.358101000
H	4.618780000	6.516182000	7.594575000
H	7.894710000	4.820118000	8.303378000
H	6.211725000	4.999751000	8.870866000
H	7.285809000	6.417037000	8.782720000
H	7.364445000	6.536518000	5.002703000
H	8.503072000	5.557312000	5.958884000
H	8.124361000	7.220266000	6.472643000
H	5.916050000	1.983917000	8.628258000
C	7.968614000	1.457375000	9.034456000
C	9.586616000	2.163514000	7.390022000
H	8.796221000	3.231111000	5.687044000
H	4.781673000	5.893459000	11.508107000
H	3.767992000	4.590887000	12.153370000
H	3.092911000	6.226538000	11.946819000
H	4.898999000	9.022599000	0.569158000
H	6.386823000	8.247898000	0.014008000
H	-0.220221000	10.508426000	5.205220000
H	1.336282000	10.492298000	4.370808000

H	-0.816327000	1.946328000	0.579878000
H	-0.223174000	1.805742000	2.240652000
H	7.729428000	0.956277000	9.975240000
C	9.289081000	1.524692000	8.593996000
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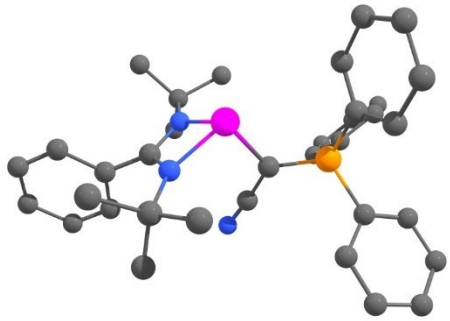

AYSi-3

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C	27.551416000	8.634578000	7.263324000
C	26.421647000	6.846860000	9.758973000
C	28.408199000	5.404512000	9.077613000
C	25.091138000	8.989479000	10.116615000
C	26.535548000	7.796388000	6.791147000
P	28.118288000	9.862550000	6.225935000
C	25.453570000	5.816719000	10.216071000
C	27.670424000	4.429918000	8.154251000
C	29.715685000	5.831475000	8.408166000
C	28.722778000	4.736004000	10.419476000
C	23.819840000	8.546756000	9.385772000
C	24.871839000	8.966024000	11.632532000
C	25.444354000	10.412874000	9.678367000
N	25.677114000	7.054683000	6.492245000
C	29.505885000	10.732816000	6.990554000
C	26.899200000	11.154152000	5.793173000
C	28.697282000	9.228941000	4.619285000
C	25.395400000	5.419607000	11.555096000
C	24.583375000	5.245574000	9.279258000
H	27.336509000	4.943138000	7.240571000
H	26.786403000	4.000896000	8.645046000
H	28.336623000	3.598173000	7.877348000
H	29.510291000	6.320995000	7.444633000
H	30.360973000	4.958690000	8.231406000
H	30.262078000	6.548816000	9.040191000
H	29.375602000	3.861724000	10.270756000
H	27.804517000	4.389885000	10.915210000
H	29.236496000	5.443462000	11.088155000
H	24.015145000	8.436386000	8.309012000
H	23.024420000	9.293935000	9.531450000
H	23.449094000	7.584926000	9.765120000
H	24.062790000	9.656783000	11.917289000
H	25.790573000	9.270555000	12.156620000
H	24.592044000	7.959349000	11.974793000
H	25.583229000	10.459229000	8.588073000
H	26.378425000	10.743489000	10.160503000

H	24.643135000	11.111792000	9.959517000
C	29.262380000	11.563806000	8.092315000
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C	25.555627000	10.776121000	5.669152000
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C	29.037863000	7.876191000	4.525093000
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H	24.641222000	5.572701000	8.236507000
H	28.240030000	11.724529000	8.441732000
C	30.325695000	12.190951000	8.734520000
C	31.875036000	11.154596000	7.195792000
H	31.003358000	9.872393000	5.691391000
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H	28.311996000	12.792077000	5.698345000
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C	29.522167000	7.363513000	3.323191000
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H	24.431850000	4.146445000	13.004632000
C	23.606719000	3.886588000	11.024829000
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H	30.134490000	12.835143000	9.595380000
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C	24.964180000	13.058745000	5.138156000
H	26.590753000	14.480231000	5.111871000
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H	22.883639000	3.130906000	11.341213000
H	32.463983000	12.477182000	8.795618000
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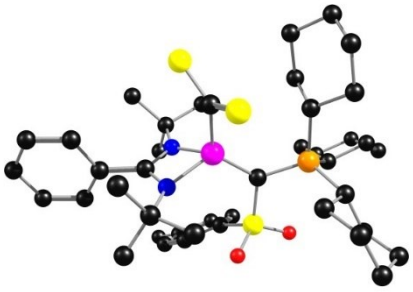

4

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O	6.989385000	7.677409000	11.781160000
C	8.351262000	9.824918000	11.397302000
P	4.153722000	10.127925000	11.857974000
Si	5.444389000	9.458442000	8.881536000

C	9.531707000	9.646984000	10.676345000
C	8.330937000	10.649995000	12.516115000
C	4.868241000	11.413318000	13.004322000
C	3.841940000	8.692455000	13.021959000
N	4.864574000	7.824449000	8.144753000
N	3.570250000	9.528829000	8.422472000
N	6.190142000	10.695135000	7.859345000
C	3.596092000	8.252515000	8.085892000
H	9.539872000	8.982329000	9.811137000
C	10.679572000	10.330269000	11.064955000
C	9.484747000	11.331905000	12.889679000
H	7.417237000	10.768246000	13.097888000
H	5.680387000	10.964211000	13.604594000
C	5.435092000	12.575162000	12.195251000
C	3.805688000	11.913527000	13.984831000
H	2.896200000	8.982468000	13.521331000
C	4.877529000	8.408557000	14.109779000
C	3.552032000	7.446827000	12.185097000
C	5.413001000	6.460345000	7.962869000
C	2.437675000	10.473674000	8.444732000
C	7.250039000	11.359420000	8.547619000
C	6.399029000	10.637452000	6.383905000
C	2.416740000	7.426740000	7.722291000
H	11.601442000	10.192991000	10.493132000
C	10.675576000	11.193390000	12.167810000
H	9.456646000	11.987585000	13.764214000
H	4.622816000	12.991370000	11.571858000
H	6.195601000	12.204721000	11.490914000
C	5.992530000	13.675532000	13.088879000
C	4.357122000	13.013863000	14.888201000
H	3.419057000	11.082912000	14.597621000
H	2.945207000	12.299743000	13.408283000
H	5.000712000	9.289309000	14.760427000
H	5.851744000	8.210337000	13.637394000
C	4.481633000	7.202026000	14.958415000
C	3.174063000	6.244145000	13.041199000
H	2.752119000	7.678301000	11.461194000
H	4.453276000	7.209922000	11.599301000
C	6.817882000	6.571675000	7.362706000
C	5.471058000	5.746909000	9.315240000
C	4.595578000	5.610275000	6.983388000
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H	6.868470000	13.287975000	13.641293000
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C	4.944126000	14.167387000	14.081272000
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H	3.567694000	13.381180000	15.564429000
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H	5.263804000	6.998648000	15.708330000
C	4.238707000	5.968317000	14.096643000
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H	7.247504000	5.563670000	7.268431000
H	6.777116000	7.012671000	6.355527000
H	7.478784000	7.173615000	7.993953000
H	6.100592000	6.289048000	10.032231000
H	4.461925000	5.649673000	9.742926000

H	5.884110000	4.734121000	9.190863000
H	3.620532000	5.302150000	7.377798000
H	4.440048000	6.130546000	6.027041000
H	5.169191000	4.695336000	6.775328000
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H	1.835524000	9.949642000	10.458188000
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H	7.909760000	9.070236000	6.522134000
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H	5.464364000	9.842827000	4.612106000
H	5.402221000	8.731721000	5.996577000
H	7.040033000	12.719064000	6.270264000
H	6.501414000	12.031635000	4.720926000
H	5.300085000	12.471448000	5.963675000
H	2.108985000	6.734293000	9.741332000
C	0.672501000	5.884512000	8.369178000
C	0.888816000	6.561970000	6.062528000
H	2.498425000	7.933735000	5.626354000
H	11.931079000	12.183459000	13.621991000
H	12.820876000	11.432990000	12.272160000
H	11.922322000	12.941144000	12.018197000
H	5.372243000	14.928790000	14.753749000
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H	5.181294000	5.690907000	13.592880000
H	3.947297000	5.109760000	14.723971000
H	5.363876000	13.202503000	8.182971000
H	5.694147000	13.827906000	9.799278000
C	6.671398000	14.944299000	8.241853000
C	8.961564000	14.465662000	9.154314000
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C	0.235969000	5.820401000	7.046749000
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H	6.999603000	14.785380000	7.199463000
C	7.840151000	15.492467000	9.051770000
H	9.372605000	14.273915000	8.146939000
H	9.792646000	14.856994000	9.764027000
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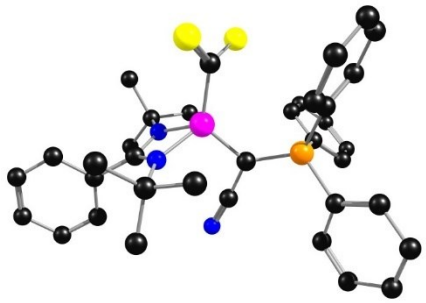

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P	0.273289000	6.946554000	3.708021000
N	4.290820000	9.009229000	4.446841000
C	2.886791000	6.293000000	3.962555000
N	4.326481000	8.482959000	2.362156000
C	-0.397573000	6.831137000	5.392103000
C	-1.178622000	5.751108000	5.815529000
H	-1.405192000	4.932889000	5.128736000
C	-1.664231000	5.720495000	7.122256000
H	-2.268469000	4.873723000	7.455649000
C	-1.378664000	6.765772000	7.998635000
H	-1.760187000	6.737758000	9.022218000
C	-0.608721000	7.848899000	7.571008000
H	-0.390920000	8.673275000	8.253856000
C	-0.113563000	7.884462000	6.271528000
H	0.472556000	8.738890000	5.916275000
C	5.091760000	8.664470000	3.434953000
C	6.554652000	8.463036000	3.508372000
C	7.042960000	7.188149000	3.814432000
H	6.337533000	6.368967000	3.979938000
C	8.416553000	6.989344000	3.914685000
H	8.801941000	5.996528000	4.157068000
C	9.297484000	8.052166000	3.710149000
H	10.374956000	7.890953000	3.791439000
C	8.805720000	9.319649000	3.401982000
H	9.494426000	10.151795000	3.240322000
C	7.431716000	9.529519000	3.300422000
H	7.037451000	10.519999000	3.062239000
C	4.559445000	9.405968000	5.835157000
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H	4.937459000	11.265270000	6.899697000
H	5.677899000	11.191241000	5.280109000
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C	3.307261000	9.049616000	6.634787000
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H	3.112547000	7.967624000	6.591570000
C	5.751086000	8.663994000	6.438881000
H	5.793977000	8.893231000	7.513831000
H	5.632665000	7.576530000	6.325101000
H	6.710015000	8.963508000	5.997128000
C	4.642395000	8.098716000	0.981282000
C	5.412489000	6.777900000	0.933214000
H	4.902682000	6.009818000	1.534112000
H	5.470377000	6.427734000	-0.108290000
H	6.440104000	6.887567000	1.304206000
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C	3.296047000	7.924021000	0.279744000
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C	5.423608000	9.226577000	0.305104000
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H	5.584363000	8.991001000	-0.757899000
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C	-0.102737000	5.347168000	2.928232000
C	-1.101427000	5.256984000	1.951855000
C	0.597528000	4.195494000	3.317481000
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H	-1.651744000	6.150479000	1.649380000
C	0.301994000	2.972281000	2.722573000
H	1.380763000	4.249009000	4.076187000
C	-0.690649000	2.885963000	1.746253000
H	-2.170751000	3.964462000	0.600226000

H	0.855116000	2.080248000	3.024790000
H	-0.917966000	1.923365000	1.282030000
C	-0.678731000	8.206108000	2.840850000
C	-1.840415000	8.742900000	3.406033000
C	-0.245430000	8.632845000	1.580979000
C	-2.544991000	9.727281000	2.721360000
H	-2.174771000	8.414316000	4.391693000
C	-0.953155000	9.621702000	0.905756000
H	0.658394000	8.211142000	1.138783000
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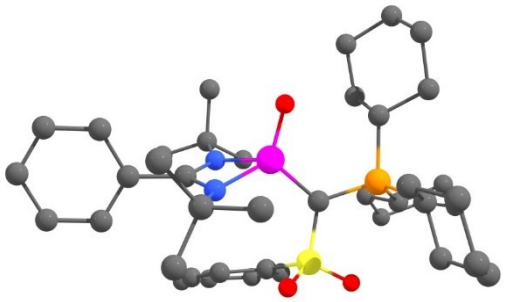

6

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O	2.019596000	2.587691000	5.977038000
C	2.486625000	4.522914000	7.627619000
P	2.274009000	5.692507000	3.549641000
Si	4.758796000	4.167284000	4.692798000
C	1.956176000	5.661134000	8.229507000
C	3.378541000	3.710697000	8.321879000
C	3.611430000	6.351313000	2.475975000
C	1.203089000	7.040107000	4.199011000
C	1.220103000	4.703058000	2.399971000
N	5.148800000	2.541688000	5.499235000
N	5.797479000	4.455052000	6.237142000
C	5.973058000	3.145195000	6.358466000
H	1.197113000	6.240476000	7.702909000
C	2.379987000	6.022926000	9.505170000
C	3.790010000	4.079734000	9.598112000
H	3.716301000	2.785461000	7.852723000
H	4.305915000	5.481778000	2.445434000
C	4.429752000	7.466699000	3.129973000
C	3.235389000	6.734175000	1.042545000
H	0.377865000	6.474160000	4.659959000
C	1.857734000	7.851308000	5.317792000
C	0.626759000	7.961151000	3.123267000
H	1.022337000	5.392853000	1.559464000
C	-0.132542000	4.241721000	2.944167000
C	2.026674000	3.511280000	1.878293000
C	5.050470000	1.145375000	5.058313000

C	6.441899000	5.623212000	6.834896000
C	6.974814000	2.471670000	7.220167000
H	1.965716000	6.919387000	9.974304000
C	3.315789000	5.250834000	10.204029000
H	4.490013000	3.443271000	10.146954000
H	3.846443000	8.404211000	3.165663000
H	4.675886000	7.201110000	4.167414000
C	5.710275000	7.691239000	2.335201000
C	4.506463000	7.003603000	0.236764000
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H	2.592079000	7.631165000	1.029095000
H	2.297718000	7.176111000	6.064157000
H	2.688379000	8.451704000	4.915449000
C	0.831745000	8.782948000	5.951777000
C	-0.391538000	8.913526000	3.747427000
H	1.437741000	8.547758000	2.658520000
H	0.151706000	7.382818000	2.315021000
H	0.022869000	3.597915000	3.821833000
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C	-0.907081000	3.484352000	1.869934000
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H	2.243836000	2.853072000	2.733239000
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C	6.411806000	0.614439000	4.603306000
C	5.344086000	6.671441000	7.031846000
C	7.078799000	5.343901000	8.195670000
C	7.491351000	6.139922000	5.844855000
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C	8.312332000	2.466804000	6.808531000
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H	6.318156000	8.479040000	2.809726000
H	6.292334000	6.754597000	2.373296000
C	5.394654000	8.056088000	0.889916000
H	5.071282000	6.059215000	0.150409000
H	4.238093000	7.307232000	-0.788451000
H	0.040271000	8.177059000	6.429114000
H	1.302031000	9.374974000	6.753807000
C	0.205773000	9.703091000	4.907978000
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H	7.396663000	6.301458000	8.634498000
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C	7.592110000	1.248434000	9.209786000
C	9.281729000	1.852654000	7.595556000
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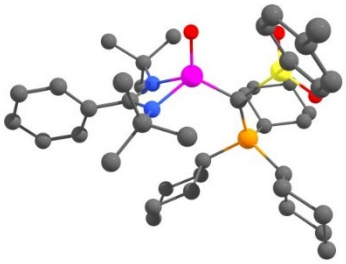

6_conformer

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C	-0.003312000	4.454613000	4.672875000
C	1.061595000	6.500658000	6.474919000
N	4.828646000	2.614854000	5.122638000
N	5.278686000	4.141611000	6.576724000
C	5.441638000	2.845411000	6.279799000
H	1.155668000	5.110699000	1.258051000
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C	-2.472051000	4.062890000	4.683326000
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C	7.456549000	1.412557000	6.670089000
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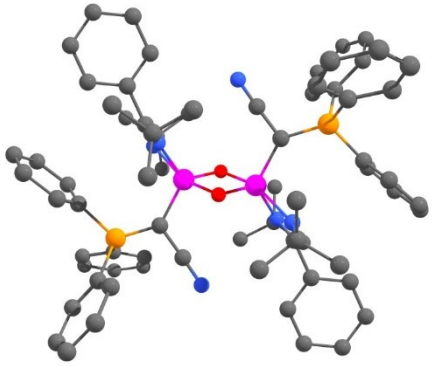

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C	17.174782000	17.120437000	21.910606000
H	18.191241000	15.627323000	23.096829000
H	15.049009000	14.499876000	27.489753000
C	13.908785000	12.754847000	26.917741000
H	12.744736000	11.144189000	26.067518000
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C	10.342157000	18.266679000	23.395739000
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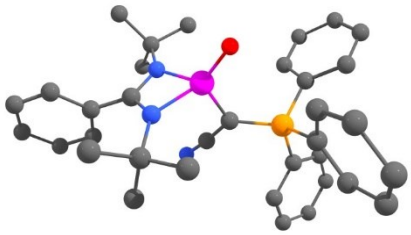

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N	13.525670000	12.916391000	18.828212000
C	12.487297000	13.195894000	18.045244000
P	12.305999000	13.580770000	23.009694000
C	11.987581000	15.033306000	20.713212000
C	9.990376000	12.679759000	18.256063000
C	14.937603000	13.294799000	18.762363000
C	12.527468000	13.920596000	16.753133000
C	13.798102000	12.738525000	23.629609000
C	10.906524000	12.642456000	23.692767000
C	12.269252000	15.198826000	23.828128000
N	11.810213000	16.016880000	20.101429000
C	9.249362000	12.092741000	19.457603000
C	9.854515000	11.734666000	17.060071000
C	9.415584000	14.059327000	17.925599000

C	15.607967000	12.623989000	17.561706000
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C	12.778452000	13.241941000	15.557584000
C	12.311334000	15.304215000	16.748504000
C	14.639401000	13.373263000	24.552615000
C	14.097821000	11.444068000	23.174919000
C	11.055660000	11.714965000	24.727240000
C	9.636800000	12.912549000	23.171631000
C	11.477373000	15.416468000	24.960337000
C	13.083729000	16.228120000	23.336984000
H	9.296925000	12.786399000	20.309110000
H	8.191970000	11.921181000	19.209541000
H	9.704438000	11.141473000	19.772928000
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H	8.793913000	11.606576000	16.795088000
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H	15.460553000	11.534260000	17.599269000
H	15.202038000	13.001936000	16.612791000
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H	16.173024000	15.075042000	18.814267000
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H	15.116571000	13.260988000	20.931228000
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C	15.783312000	12.723500000	25.012544000
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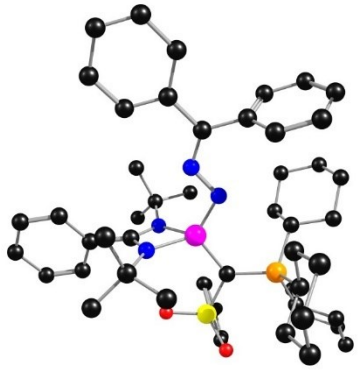

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C	2.717990000	12.686715000	7.645003000
C	3.185886000	7.001541000	7.324723000
O	3.758450000	12.078838000	1.619833000
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C	5.864789000	12.788320000	2.961865000
C	5.882593000	9.844213000	1.011927000
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C	5.783090000	7.810019000	3.285876000
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C	3.026431000	13.999411000	7.270879000
C	2.564372000	6.876717000	8.655182000
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C	6.709502000	12.678463000	4.064457000
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C	7.336192000	10.122724000	1.408977000
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H	1.753145000	11.410049000	9.095657000
C	1.575696000	13.503112000	9.606095000
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C	6.591616000	9.741371000	-1.399742000
H	6.276229000	8.028369000	-0.119771000
H	4.795134000	8.864390000	-0.606642000
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C	5.075597000	3.851932000	6.346227000
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H	1.705365000	7.979622000	-0.567863000
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H	6.973282000	4.619240000	2.693705000
C	7.744703000	5.884466000	4.279657000
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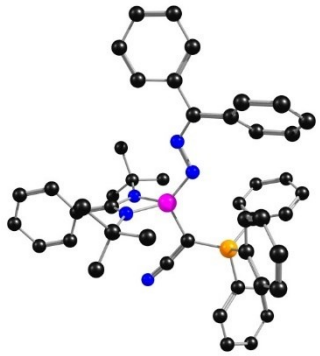

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C	9.895442000	2.696526000	10.298469000

C	8.834149000	4.958142000	8.785938000
Si	9.462954000	2.891505000	5.687148000
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C	6.950906000	1.678201000	9.959607000
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C	10.288311000	1.364194000	10.489412000
C	10.158419000	3.648610000	11.288799000
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C	7.783327000	5.550959000	9.493947000
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N	10.942332000	2.893457000	4.590663000
N	9.553725000	1.265973000	4.786050000
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H	7.654797000	1.418642000	10.752937000
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C	5.127606000	2.365125000	7.956996000
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H	9.860850000	4.688647000	11.140381000
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C	8.334924000	-0.408851000	3.482455000
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H	3.710163000	1.156559000	9.051371000
H	11.704529000	1.650846000	13.571791000
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H	10.571025000	-1.383397000	4.711208000
H	7.044465000	1.016166000	5.458490000
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C	13.315068000	-0.770428000	1.870570000
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H	7.137986000	6.289899000	6.220492000
C	5.138041000	6.264558000	7.031618000
C	3.483864000	5.074304000	5.747145000
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H	5.044367000	6.656024000	2.855008000
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C	7.051966000	4.749033000	0.147749000
H	7.985251000	3.710906000	1.802794000
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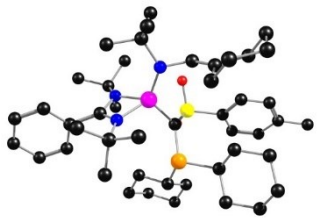

9

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S	6.595994000	9.245056000	11.313968000
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C	5.461148000	10.137970000	10.407344000
O	6.106022000	8.780017000	12.630867000
C	8.009890000	10.261230000	11.723144000
P	4.646668000	11.664609000	10.880635000
Si	4.859641000	9.173182000	9.011120000

C	8.865957000	10.669036000	10.704454000
C	8.268677000	10.607365000	13.044982000
C	5.997199000	12.922666000	11.156711000
C	3.888295000	11.479550000	12.585490000
N	3.790738000	7.679652000	9.471370000
N	3.084228000	9.540533000	8.626173000
N	5.826443000	8.995702000	7.580088000
C	2.701847000	8.371960000	9.152911000
H	8.656696000	10.356627000	9.683392000
C	9.962847000	11.464234000	11.007051000
C	9.365580000	11.416973000	13.335370000
H	7.610844000	10.236632000	13.831483000
H	6.726387000	12.545874000	11.894084000
C	6.725083000	13.164895000	9.837131000
C	5.416731000	14.238420000	11.678824000
H	3.245393000	12.379223000	12.663033000
C	4.806460000	11.447570000	13.804950000
C	2.969837000	10.258806000	12.569350000
C	3.909190000	6.377733000	10.170711000
C	2.277789000	10.632100000	8.043437000
C	7.165523000	9.495354000	7.670239000
C	5.640468000	8.061745000	6.424693000
C	1.298867000	7.923244000	9.335497000
H	10.632582000	11.784055000	10.203635000
C	10.222170000	11.867379000	12.325594000
H	9.563819000	11.699268000	14.372906000
H	5.982257000	13.497797000	9.087803000
H	7.135351000	12.215704000	9.462784000
C	7.813349000	14.222114000	9.969191000
C	6.500894000	15.303670000	11.823465000
H	4.911052000	14.089756000	12.645708000
H	4.640593000	14.591246000	10.973889000
H	5.445637000	12.343889000	13.838672000
H	5.467104000	10.574647000	13.711254000
C	4.005926000	11.323948000	15.098849000
C	2.184857000	10.106283000	13.867366000
H	2.284753000	10.335407000	11.709601000
H	3.595258000	9.366987000	12.404064000
C	5.266291000	5.776897000	9.808162000
C	3.821727000	6.594888000	11.682033000
C	2.831531000	5.379648000	9.733289000
C	1.373144000	10.127205000	6.914806000
C	1.432650000	11.326156000	9.112618000
C	3.268142000	11.627340000	7.449525000
H	7.880683000	8.830649000	8.169578000
C	7.612795000	10.663721000	7.178513000
C	6.725130000	6.978007000	6.451783000
C	4.272605000	7.387912000	6.447389000
C	5.746684000	8.839051000	5.111077000
C	0.639493000	8.136779000	10.548413000
C	0.646851000	7.247875000	8.298826000
C	11.380290000	12.770523000	12.631105000
H	8.596583000	13.844242000	10.649728000
H	8.301937000	14.389457000	8.993659000
C	7.250863000	15.529812000	10.515190000
H	7.217250000	14.979294000	12.600095000
H	6.059866000	16.248590000	12.181981000
H	3.379955000	12.225494000	15.236891000

H	4.689309000	11.285424000	15.963556000
C	3.112832000	10.088169000	15.076766000
H	1.577379000	9.184424000	13.839263000
H	1.472161000	10.945813000	13.966669000
H	5.416682000	4.856178000	10.390089000
H	5.302528000	5.506097000	8.742608000
H	6.086740000	6.469661000	10.036444000
H	4.614413000	7.266522000	12.039683000
H	2.845524000	7.020206000	11.958538000
H	3.926134000	5.629649000	12.200468000
H	1.834192000	5.618388000	10.121417000
H	2.773425000	5.298055000	8.637438000
H	3.109083000	4.390811000	10.126370000
H	0.546882000	9.508116000	7.285468000
H	0.931201000	10.992529000	6.399224000
H	1.944741000	9.551944000	6.171087000
H	2.089686000	11.744497000	9.888437000
H	0.861575000	12.147871000	8.654632000
H	0.713981000	10.632539000	9.571389000
H	3.973201000	11.972923000	8.220455000
H	3.826153000	11.164592000	6.624462000
H	2.729807000	12.501632000	7.056746000
C	6.768510000	11.703479000	6.502935000
C	9.070279000	11.027020000	7.281353000
H	6.745801000	6.472489000	7.426997000
H	6.532064000	6.228494000	5.669410000
H	7.721952000	7.403346000	6.268891000
H	3.466540000	8.133060000	6.471176000
H	4.153192000	6.792856000	5.530922000
H	4.158915000	6.715719000	7.304406000
H	6.714215000	9.350339000	5.030179000
H	5.657394000	8.148682000	4.258537000
H	4.945466000	9.589012000	5.029791000
H	1.149759000	8.659587000	11.358023000
C	-0.664401000	7.676669000	10.720957000
C	-0.654517000	6.789309000	8.476475000
H	1.169043000	7.068736000	7.356943000
H	11.583024000	12.818827000	13.710008000
H	12.297163000	12.434113000	12.123676000
H	11.176640000	13.797143000	12.283491000
H	8.055297000	16.270713000	10.655713000
H	6.556000000	15.962542000	9.772251000
H	3.750331000	9.187928000	15.026175000
H	2.529191000	10.013178000	16.009253000
H	5.748633000	11.329955000	6.370430000
H	6.696950000	12.573127000	7.179578000
C	7.363342000	12.173452000	5.173937000
C	9.644840000	11.454936000	5.930486000
H	9.173183000	11.878049000	7.981885000
H	9.648736000	10.190835000	7.703926000
H	-1.173493000	7.846102000	11.672220000
C	-1.312394000	7.002417000	9.687977000
H	-1.156746000	6.257841000	7.665186000
H	6.764086000	13.008138000	4.775626000
H	7.292765000	11.360144000	4.430826000
C	8.823015000	12.583604000	5.320898000
H	9.643292000	10.588824000	5.245035000
H	10.697065000	11.759843000	6.050037000

H	-2.333434000	6.639796000	9.826750000
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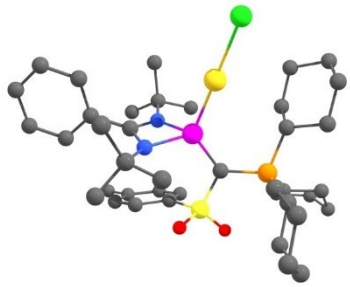
H	9.239104000	12.882139000	4.344981000



AYSi-2-AuCl

E = -3481.02731011

S	2.210043000	4.361961000	5.882109000
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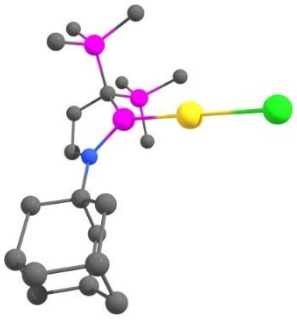
C	3.277472000	5.042219000	4.700218000
O	2.129680000	2.894606000	5.757622000
C	2.869437000	4.636553000	7.527112000
P	2.479910000	5.917055000	3.387297000
Si	4.996473000	4.411573000	4.613276000
C	2.745583000	5.889997000	8.124237000
C	3.323464000	3.549831000	8.266308000
C	3.753282000	6.651397000	2.280214000
C	1.326016000	7.219834000	3.984675000
C	1.484122000	4.821409000	2.288014000
N	5.292351000	2.758692000	5.425275000
N	5.976564000	4.646434000	6.184760000
C	6.121542000	3.326889000	6.302621000
H	2.320438000	6.722035000	7.562556000
C	3.125661000	6.061266000	9.450064000
C	3.684444000	3.730808000	9.599655000
H	3.362229000	2.568284000	7.793126000
H	4.509346000	5.841975000	2.228672000
C	4.459109000	7.867561000	2.882120000
C	3.328862000	6.939679000	0.836280000
H	0.547848000	6.616272000	4.476263000
C	1.912204000	8.123804000	5.068550000
C	0.669279000	8.051966000	2.882147000
H	1.161556000	5.478178000	1.459835000
C	0.231201000	4.228167000	2.937225000
C	2.375372000	3.712759000	1.723446000
C	5.159008000	1.355807000	4.999845000
C	6.704352000	5.761764000	6.797685000
C	7.126788000	2.630478000	7.143037000
H	3.029061000	7.047179000	9.912484000
C	3.605659000	4.986475000	10.211292000
H	4.019927000	2.872199000	10.188379000
H	3.763491000	8.723956000	2.897791000
H	4.739452000	7.668617000	3.925792000
C	5.686474000	8.236271000	2.056419000
C	4.559684000	7.311468000	0.009427000
H	2.841901000	6.066682000	0.379970000

H	2.596528000	7.764224000	0.808574000
H	2.426875000	7.513660000	5.821515000
H	2.673170000	8.793244000	4.639287000
C	0.803119000	8.962635000	5.691601000
C	-0.434647000	8.917064000	3.489275000
H	1.418889000	8.701684000	2.399048000
H	0.247873000	7.411359000	2.091670000
H	0.520692000	3.618021000	3.806264000
H	-0.422685000	5.022708000	3.326822000
C	-0.529335000	3.360528000	1.939112000
C	1.614373000	2.830189000	0.740699000
H	3.279094000	4.120984000	1.244402000
H	2.727066000	3.102824000	2.567280000
C	4.206154000	1.359385000	3.808112000
C	4.542962000	0.526043000	6.127182000
C	6.502272000	0.770510000	4.557261000
C	5.907357000	7.019347000	6.460106000
C	6.777023000	5.601820000	8.315860000
C	8.108752000	5.891186000	6.199639000
C	6.794276000	2.115649000	8.397990000
C	8.432819000	2.492494000	6.659328000
C	4.043280000	5.184595000	11.631455000
H	6.178188000	9.119285000	2.495588000
H	6.415736000	7.408261000	2.103391000
C	5.313273000	8.495577000	0.602550000
H	5.238288000	6.441585000	-0.035559000
H	4.253129000	7.528808000	-1.026316000
H	0.085517000	8.289689000	6.193483000
H	1.217900000	9.621805000	6.471630000
C	0.083677000	9.788472000	4.629108000
H	-0.893806000	9.542466000	2.706778000
H	-1.233009000	8.255457000	3.869697000
H	-1.418269000	2.931985000	2.428774000
H	-0.902603000	3.991513000	1.111407000
C	0.353045000	2.255040000	1.372358000
H	1.342377000	3.424272000	-0.150944000
H	2.274887000	2.023250000	0.385226000
H	4.639502000	1.925663000	2.968809000
H	3.247357000	1.806464000	4.103975000
H	4.028611000	0.329138000	3.467572000
H	4.421816000	-0.516683000	5.797589000
H	3.551417000	0.925579000	6.383278000
H	5.183806000	0.520571000	7.020407000
H	6.335090000	-0.208388000	4.083739000
H	7.189803000	0.618455000	5.399453000
H	6.983156000	1.429542000	3.817478000
H	5.899309000	7.183138000	5.373049000
H	6.368733000	7.899450000	6.930122000
H	4.868867000	6.931062000	6.806889000
H	7.409765000	4.753944000	8.609762000
H	5.772904000	5.454864000	8.736894000
H	7.210584000	6.511350000	8.757730000
H	8.058710000	5.925055000	5.100270000
H	8.750445000	5.050466000	6.495463000
H	8.585589000	6.816892000	6.556054000
H	5.779743000	2.237556000	8.776918000
C	7.762168000	1.473015000	9.166640000
C	9.396251000	1.847939000	7.430255000

H	8.685681000	2.877240000	5.668836000
H	5.092703000	5.522645000	11.668935000
H	3.978114000	4.251699000	12.209060000
H	3.436785000	5.948531000	12.138943000
H	4.681746000	9.401664000	0.541797000
H	6.217625000	8.701823000	0.009026000
H	-0.745647000	10.357984000	5.078446000
H	0.786934000	10.536414000	4.219580000
H	-0.205718000	1.652250000	0.638395000
H	0.639349000	1.569827000	2.190057000
H	7.496970000	1.075826000	10.149000000
C	9.063320000	1.339018000	8.685326000
H	10.412461000	1.739879000	7.044878000
H	9.820907000	0.834139000	9.289042000
Au	6.369333000	4.586262000	2.788949000
Cl	7.781794000	4.728623000	0.918918000



CAASi-AuCl

E = -2228.57331337

Si	5.829021000	3.273082000	9.530359000
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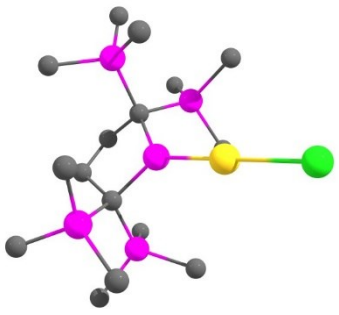
C	7.107019000	4.278859000	10.428136000
C	8.821844000	2.328927000	10.823974000
C	7.388690000	0.882804000	10.008415000
Si	7.242238000	5.946073000	9.475097000
Si	6.409832000	4.606979000	12.178408000
C	8.581554000	3.796369000	10.587847000
H	9.871531000	2.078123000	11.026772000
H	8.347973000	2.212628000	11.826870000
C	6.881295000	2.315923000	8.187775000
C	5.313668000	1.711117000	10.593402000
C	7.583779000	-0.156271000	10.021284000
C	7.409798000	5.608191000	7.626179000
C	5.826942000	7.158576000	9.720492000
C	8.833835000	6.830069000	9.983188000
C	6.728717000	3.198001000	13.405928000
C	7.231958000	6.088969000	13.005987000
C	4.547080000	4.874779000	12.200125000
H	9.138371000	4.092892000	9.676828000
H	9.042674000	4.382862000	11.402529000
H	7.966299000	2.074620000	8.312003000
H	6.913596000	3.076031000	7.403461000
C	6.120851000	1.101417000	7.596148000
H	4.463643000	2.137079000	11.134662000
H	5.864076000	1.275800000	11.459548000
C	4.718588000	0.549692000	9.721224000
H	7.466791000	-0.600905000	10.962395000

H	8.581154000	-0.365010000	9.700503000
C	6.705464000	-0.896120000	9.073488000
H	6.479213000	5.213064000	7.189564000
H	8.239154000	4.917059000	7.408764000
H	7.636008000	6.557736000	7.114715000
H	5.715959000	7.493397000	10.761917000
H	4.863254000	6.747990000	9.381044000
H	6.040172000	8.049318000	9.107142000
H	8.852751000	7.806872000	9.472824000
H	9.736515000	6.280862000	9.678761000
H	8.896983000	7.020849000	11.063005000
H	6.284631000	3.515574000	14.364279000
H	7.799784000	3.023100000	13.589690000
H	6.259896000	2.238396000	13.147186000
H	7.037419000	7.037950000	12.487311000
H	8.322134000	5.959037000	13.088581000
H	6.832782000	6.180315000	14.029006000
H	4.242579000	5.087277000	13.238629000
H	3.972367000	4.000934000	11.859994000
H	4.229860000	5.720346000	11.574050000
H	5.955982000	1.288032000	6.524990000
C	4.729002000	0.931107000	8.227766000
C	6.806202000	-0.263315000	7.691524000
H	3.661332000	0.432645000	9.999452000
C	5.337281000	-0.862300000	9.746657000
H	7.095045000	-1.922935000	9.053650000
H	4.138088000	1.843712000	8.059959000
H	4.203983000	0.135807000	7.672021000
H	6.316952000	-0.934136000	6.969278000
H	7.871439000	-0.215059000	7.401956000
H	4.629424000	-1.524971000	9.226463000
H	5.438532000	-1.261177000	10.770940000
Au	3.990266000	4.330861000	8.703577000
Cl	2.088653000	5.399166000	7.841082000



CA_2Si-AuCl

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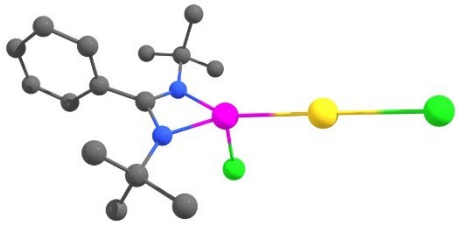
C	2.766870000	9.046486000	11.674926000
Si	0.200434000	7.149532000	9.010786000
Si	3.172001000	6.169373000	8.562161000
C	2.041786000	6.663575000	11.195726000
Si	1.929375000	10.754698000	12.000288000
Si	4.536434000	9.017622000	12.427765000

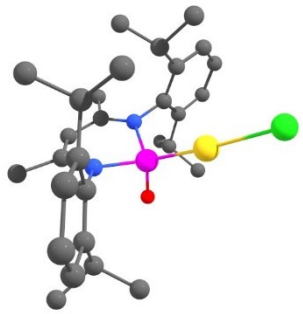
C	1.897089000	7.850955000	12.159877000
C	-1.063576000	7.427089000	10.384933000
C	-0.258501000	5.460229000	8.307556000
C	-0.029518000	8.475996000	7.700686000
C	3.010429000	4.331636000	8.932100000
C	2.874388000	6.549211000	6.746622000
C	4.971577000	6.640556000	8.892889000
H	1.270875000	5.902545000	11.403488000
H	3.005803000	6.165658000	11.392476000
C	0.484519000	11.021670000	10.812718000
C	3.102940000	12.191628000	11.705240000
C	1.217034000	10.776290000	13.741749000
C	4.584721000	9.855150000	14.117248000
C	5.078553000	7.245014000	12.785255000
C	5.790775000	9.813558000	11.278128000
H	2.153235000	7.545283000	13.188272000
H	0.835392000	8.146570000	12.197652000
H	-1.004763000	8.420770000	10.848935000
H	-0.980220000	6.671452000	11.181105000
H	-2.069767000	7.329619000	9.945783000
H	-0.189168000	4.678440000	9.079957000
H	0.349531000	5.148146000	7.447356000
H	-1.308424000	5.502050000	7.974798000
H	-1.028319000	8.375178000	7.246160000
H	0.717336000	8.413865000	6.896642000
H	0.037934000	9.486347000	8.132980000
H	2.011697000	3.935662000	8.704265000
H	3.229663000	4.119492000	9.990072000
H	3.743251000	3.776613000	8.324477000
H	3.603106000	5.979677000	6.147504000
H	3.047906000	7.618769000	6.545305000
H	1.869744000	6.288808000	6.386610000
H	5.620574000	5.975416000	8.299828000
H	5.268622000	6.529274000	9.945144000
H	5.191956000	7.672447000	8.574035000
H	-0.031208000	11.954012000	11.095685000
H	-0.262373000	10.216070000	10.843203000
H	0.823768000	11.145930000	9.771301000
H	2.552672000	13.131355000	11.873879000
H	3.449089000	12.196591000	10.658954000
H	3.984719000	12.198756000	12.360369000
H	1.988450000	10.706268000	14.520397000
H	0.505215000	9.949320000	13.889493000
H	0.665772000	11.718418000	13.892830000
H	3.896949000	9.362426000	14.822063000
H	4.345732000	10.927243000	14.096800000
H	5.603988000	9.749347000	14.523045000
H	6.058237000	7.284657000	13.288692000
H	5.198508000	6.625572000	11.886279000
H	4.382680000	6.730451000	13.465591000
H	6.768831000	9.869758000	11.782722000
H	5.505479000	10.831149000	10.976075000
H	5.925477000	9.224402000	10.357804000
Au	3.415919000	10.251906000	8.205832000
Cl	4.116790000	11.696197000	6.529433000



Roesky-AuCl

E = -2038.71458752

N	-2.158328000	10.651523000	2.130919000
Si	-0.989607000	9.198083000	2.221679000
C	-1.261080000	11.452701000	2.709986000
C	-3.213417000	10.923869000	1.129872000
N	-0.364107000	10.653956000	3.286249000
Cl	-2.032780000	8.157364000	3.792686000
C	-1.323095000	12.919469000	2.778776000
C	-4.089866000	12.090957000	1.524728000
C	-2.594099000	11.057661000	-0.219412000
C	-4.120286000	9.650279000	1.185366000
C	0.701217000	10.927334000	4.274065000
C	-0.617860000	13.516705000	1.735501000
C	-1.948888000	13.709104000	3.739204000
H	-3.546129000	12.942574000	1.529859000
H	-4.469289000	11.931164000	2.447994000
H	-4.847003000	12.180958000	0.861933000
H	-2.059852000	10.226447000	-0.430972000
H	-1.982624000	11.862184000	-0.234426000
H	-3.319118000	11.176368000	-0.913296000
H	-4.799374000	9.689703000	0.438184000
H	-4.599931000	9.618485000	2.074581000
H	-3.550517000	8.823379000	1.080174000
C	1.584876000	12.084060000	3.862858000
C	0.090101000	11.077428000	5.624238000
C	1.598013000	9.646644000	4.223249000
H	-0.173933000	12.955996000	1.053518000
C	-0.540612000	14.903066000	1.653164000
C	-1.870924000	15.095256000	3.654399000
H	-2.448593000	13.284932000	4.477872000
H	1.047825000	12.940018000	3.854342000
H	1.957033000	11.913100000	2.939170000
H	2.347157000	12.174171000	4.520364000
H	-0.448940000	10.251924000	5.845214000
H	-0.515342000	11.886589000	5.636224000
H	0.820383000	11.196790000	6.313066000
H	2.282689000	9.687079000	4.965840000
H	2.072019000	9.603303000	3.331819000
H	1.021655000	8.825994000	4.340719000
H	-0.040358000	15.327617000	0.913770000
C	-1.167416000	15.692196000	2.613475000
H	-2.315343000	15.655777000	4.337227000
H	-1.111163000	16.677858000	2.555020000
Au	-0.038499000	7.159171000	1.148699000
Cl	0.844866000	5.244518000	0.165589000

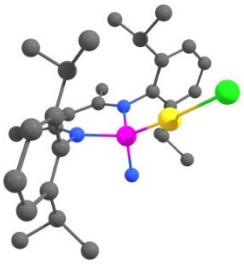


NacNac-SiOH-AuCl

E = -2197.88168406

Si	3.558419000	4.999660000	2.366204000
N	3.802686000	3.654808000	1.156868000
N	3.734646000	6.377238000	1.176677000
O	5.066462000	5.044532000	3.112408000
C	4.543167000	3.797172000	0.051592000
C	3.229549000	2.373598000	1.478279000
C	4.458823000	6.281794000	0.057456000
C	3.190979000	7.650233000	1.578387000
H	5.014956000	5.014322000	4.072699000
C	4.954891000	2.575594000	-0.707206000
C	4.924141000	5.053161000	-0.429161000
C	3.939788000	1.468661000	2.289290000
C	1.947096000	2.072198000	0.977514000
C	4.776569000	7.522410000	-0.716395000
C	4.004396000	8.570064000	2.267789000
C	1.839141000	7.927683000	1.282742000
H	5.594478000	1.942026000	-0.074557000
H	5.501736000	2.843670000	-1.618330000
H	4.081628000	1.963687000	-0.972392000
H	5.538138000	5.076330000	-1.327293000
C	3.349197000	0.231245000	2.562767000
C	5.282293000	1.808627000	2.905459000
C	1.404640000	0.820061000	1.275995000
C	1.156499000	3.052007000	0.132610000
H	5.503423000	8.133028000	-0.160462000
H	5.200202000	7.274213000	-1.696318000
H	3.882049000	8.146502000	-0.848188000
C	3.452279000	9.811682000	2.599241000
C	5.413911000	8.243186000	2.723302000
C	1.338988000	9.181890000	1.639189000
C	0.946419000	6.904126000	0.606159000
H	3.880588000	-0.485957000	3.192676000
C	2.098047000	-0.097091000	2.056701000
H	5.612059000	2.772208000	2.491822000
C	6.354862000	0.767510000	2.590297000
C	5.130426000	2.003627000	4.415721000
H	0.412891000	0.563769000	0.897141000
H	1.681494000	4.017787000	0.173762000
C	-0.248672000	3.273269000	0.687753000
C	1.108090000	2.618525000	-1.333454000
H	4.064613000	10.542158000	3.133010000
C	2.138574000	10.123011000	2.278365000
H	5.697529000	7.270967000	2.296124000
C	6.440956000	9.283063000	2.277667000
C	5.438648000	8.077662000	4.244862000
H	0.297290000	9.422456000	1.424423000

H	1.296658000	5.915395000	0.945199000
C	-0.511781000	7.015489000	1.036861000
C	1.078347000	6.943369000	-0.916838000
H	1.653725000	-1.069034000	2.283021000
H	6.117102000	-0.212757000	3.032021000
H	7.327456000	1.083937000	2.997625000
H	6.475877000	0.618830000	1.506098000
H	4.334494000	2.727802000	4.646540000
H	6.072403000	2.363085000	4.859163000
H	4.862086000	1.058793000	4.914447000
H	-0.848778000	2.350767000	0.658513000
H	-0.779917000	4.024389000	0.084180000
H	-0.220619000	3.627961000	1.729444000
H	2.113518000	2.520299000	-1.769293000
H	0.554561000	3.356213000	-1.935179000
H	0.600032000	1.647152000	-1.443263000
H	1.725029000	11.097685000	2.547402000
H	6.255000000	10.264720000	2.740480000
H	7.454509000	8.969562000	2.571368000
H	6.437519000	9.430891000	1.186839000
H	4.676984000	7.358262000	4.578071000
H	6.425066000	7.722166000	4.581358000
H	5.231379000	9.033275000	4.752045000
H	-0.981222000	7.945328000	0.679348000
H	-1.090529000	6.181625000	0.615294000
H	-0.610094000	6.964765000	2.131584000
H	2.102403000	6.724552000	-1.252332000
H	0.415441000	6.194011000	-1.377314000
H	0.795132000	7.932145000	-1.312210000
Au	1.653140000	4.945117000	3.581051000
Cl	-0.380759000	4.931976000	4.734005000



NacNac-SiNH$_2$-AuCl

E = -2178.02526035

Si	1.647495000	5.002247000	6.959501000
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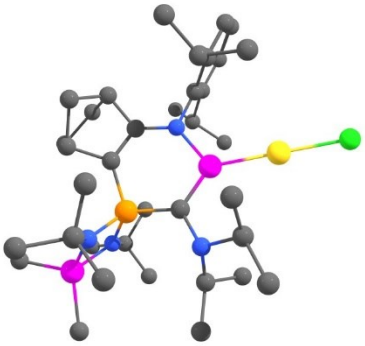
N	1.898128000	3.632522000	5.743734000
N	3.100197000	5.002891000	7.886750000
C	2.638516000	6.248659000	4.640587000
C	1.343288000	7.654588000	6.102934000
C	2.639741000	3.757103000	4.640446000
C	1.343599000	2.350470000	6.101299000
H	4.046002000	5.003369000	7.525155000
H	3.063708000	5.001856000	8.897226000
C	3.025367000	7.473875000	3.871213000
C	3.069491000	5.003095000	4.165623000
C	0.011898000	7.934097000	5.725003000
C	2.113847000	8.588092000	6.823450000
C	3.028164000	2.532164000	3.871429000

C	0.012950000	2.071079000	5.720728000
C	2.112702000	1.416885000	6.823205000
H	2.176607000	8.161711000	3.760834000
H	3.415164000	7.207871000	2.881802000
H	3.805048000	8.024415000	4.419120000
H	3.687297000	5.003456000	3.269583000
C	-0.518744000	9.181904000	6.057542000
C	-0.824927000	6.932540000	4.954512000
C	1.532719000	9.822798000	7.131218000
C	3.520993000	8.304847000	7.312431000
H	2.179920000	1.843867000	3.759958000
H	3.419053000	2.798395000	2.882511000
H	3.807425000	1.982012000	4.420348000
C	-0.518466000	0.823321000	6.052186000
C	-0.822231000	3.072628000	4.948451000
C	1.530870000	0.182228000	7.129844000
C	3.518950000	1.700131000	7.314696000
H	-1.546421000	9.416285000	5.776329000
C	0.233123000	10.123932000	6.749646000
H	-0.414854000	5.938792000	5.185649000
C	-0.697824000	7.140776000	3.444352000
C	-2.286899000	6.921212000	5.388061000
H	2.113278000	10.559475000	7.691413000
H	3.822767000	7.326480000	6.912426000
C	3.538989000	8.192445000	8.837787000
C	4.530144000	9.350186000	6.837009000
H	-1.545606000	0.589014000	5.768904000
C	0.231968000	-0.118766000	6.745773000
H	-0.410684000	4.066168000	5.177788000
C	-0.695218000	2.861476000	3.438683000
C	-2.284257000	3.086737000	5.381784000
H	2.110288000	-0.554527000	7.691117000
H	3.821311000	2.678589000	6.915361000
C	3.534240000	1.812364000	8.840092000
C	4.528984000	0.654981000	6.840768000
H	-0.202534000	11.093069000	7.003180000
H	-1.049226000	8.144188000	3.154585000
H	-1.306887000	6.400323000	2.902501000
H	0.339607000	7.033610000	3.095644000
H	-2.800840000	7.862337000	5.137806000
H	-2.386229000	6.740332000	6.469078000
H	-2.824343000	6.116406000	4.865752000
H	3.292688000	9.157409000	9.308060000
H	4.536244000	7.890084000	9.195241000
H	2.806375000	7.451974000	9.185956000
H	4.526164000	9.466055000	5.742571000
H	5.549305000	9.069074000	7.144806000
H	4.320098000	10.340749000	7.269172000
H	-0.204271000	-1.087861000	6.998465000
H	-1.048156000	1.858098000	3.150667000
H	-1.302991000	3.601914000	2.895370000
H	0.342461000	2.966312000	3.090002000
H	-2.799298000	2.145685000	5.133542000
H	-2.383525000	3.269969000	6.462419000
H	-2.820659000	3.891020000	4.857574000
H	3.287407000	0.847281000	9.309843000
H	4.530760000	2.115012000	9.199344000
H	2.800725000	2.552506000	9.187112000

H	4.527001000	0.539616000	5.746268000
H	5.547575000	0.935974000	7.150556000
H	4.318140000	-0.335767000	7.272122000
Au	-0.339457000	5.000985000	8.045829000
Cl	-2.452759000	4.999899000	9.057095000



D-AuCl

E = -3141.37195577

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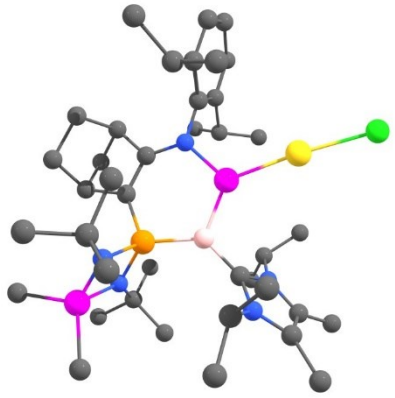
N	6.325402000	18.264252000	4.731943000
C	4.189990000	16.344742000	5.476375000
C	5.375628000	16.274744000	2.939402000
Si	5.675964000	19.801645000	4.153768000
C	2.997080000	19.080941000	3.090988000
C	7.528879000	17.887177000	5.481061000
N	4.128721000	16.815808000	6.829554000
Si	3.339203000	14.856051000	4.963589000
C	4.838828000	15.048076000	2.646249000
C	6.348279000	16.596985000	1.813155000
C	6.593106000	20.515697000	2.687839000
C	5.402921000	21.131627000	5.431662000
C	2.023678000	19.747632000	4.069660000
C	3.250809000	20.039978000	1.925673000
C	2.361654000	17.796295000	2.560427000
C	7.853941000	16.411950000	5.250115000
C	7.304777000	18.152168000	6.971348000
C	8.689645000	18.740943000	4.971405000
C	3.153896000	17.914268000	6.988570000
C	4.161809000	15.759342000	7.863336000
N	3.889375000	14.370837000	3.345450000
C	5.449751000	14.598645000	1.334355000
C	5.524669000	16.896687000	0.537904000
H	7.101615000	17.355625000	2.064074000
C	6.860549000	15.184779000	1.490271000
H	6.701350000	19.767132000	1.889608000
H	7.598877000	20.848868000	2.987345000
H	6.067138000	21.389173000	2.273201000
H	4.825719000	21.965702000	5.001109000
H	6.364068000	21.544720000	5.777300000
H	4.857854000	20.741400000	6.301445000
H	1.710110000	19.047683000	4.855456000
H	1.118514000	20.088398000	3.544137000
H	2.488841000	20.621247000	4.551299000
H	3.639313000	21.006339000	2.285392000
H	2.316403000	20.244546000	1.382026000

H	3.980082000	19.620459000	1.217880000
H	2.997275000	17.311454000	1.808208000
H	1.390191000	18.023097000	2.097371000
H	2.184676000	17.078650000	3.375351000
H	7.025724000	15.767067000	5.574129000
H	8.750187000	16.130741000	5.822560000
H	8.046495000	16.213053000	4.185956000
H	7.155214000	19.228371000	7.151893000
H	8.167037000	17.822692000	7.571492000
H	6.399424000	17.624828000	7.303187000
H	8.860195000	18.575074000	3.896893000
H	9.615040000	18.493357000	5.512244000
H	8.494554000	19.814061000	5.131821000
H	3.194429000	18.415426000	6.013611000
C	1.718914000	17.432205000	7.176641000
C	3.543871000	18.996089000	7.994189000
H	3.250826000	15.128876000	7.789769000
C	5.365599000	14.839235000	7.690754000
C	4.195287000	16.312851000	9.281896000
C	3.488212000	13.064445000	2.894372000
H	5.354317000	13.527747000	1.119987000
C	4.864092000	15.530063000	0.235335000
H	6.185026000	17.213627000	-0.284250000
H	4.798151000	17.702839000	0.703712000
H	7.452456000	15.132592000	0.562475000
H	7.424145000	14.731058000	2.318674000
H	1.442975000	16.698111000	6.402581000
H	1.014481000	18.275865000	7.109356000
H	1.565127000	16.952690000	8.154780000
H	3.289676000	18.751745000	9.032792000
H	3.007512000	19.925484000	7.744602000
H	4.622917000	19.197702000	7.945997000
H	5.412353000	14.376115000	6.696441000
H	5.307263000	14.024347000	8.426436000
H	6.304557000	15.389022000	7.855268000
H	5.037168000	17.008034000	9.423152000
H	4.325594000	15.474852000	9.981690000
H	3.267637000	16.823247000	9.565740000
C	2.348419000	12.939324000	2.079454000
C	4.230200000	11.943608000	3.313559000
H	5.143736000	15.154243000	-0.760038000
H	3.766440000	15.561235000	0.271994000
C	1.961282000	11.655612000	1.686181000
C	1.523597000	14.146636000	1.682871000
C	3.806238000	10.681496000	2.889432000
C	5.448052000	12.068704000	4.209044000
H	1.072812000	11.529895000	1.063571000
C	2.682516000	10.535633000	2.084482000
H	2.141884000	15.035480000	1.875568000
C	0.278146000	14.260016000	2.563776000
C	1.158223000	14.153447000	0.200726000
H	4.360806000	9.795165000	3.206831000
H	5.581138000	13.136100000	4.446129000
C	6.718679000	11.606627000	3.495262000
C	5.247508000	11.330082000	5.532130000
H	2.360488000	9.539657000	1.771946000
H	-0.389212000	13.396650000	2.414071000
H	-0.287497000	15.175086000	2.326428000

H	0.541898000	14.281118000	3.632859000
H	0.459543000	13.340997000	-0.052598000
H	2.047525000	14.039583000	-0.437797000
H	0.663402000	15.100274000	-0.066208000
H	6.669295000	10.535367000	3.243675000
H	7.599805000	11.756828000	4.138577000
H	6.882126000	12.161110000	2.558915000
H	4.333325000	11.670916000	6.042543000
H	6.103367000	11.501786000	6.203497000
H	5.156176000	10.243618000	5.377397000
Au	1.983564000	13.407563000	6.046360000
Cl	0.611532000	11.916718000	7.191836000



BoraylideSi-AuCl

E = -3376.64599352

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N	-3.412784000	14.483824000	7.127987000
P	-2.791530000	11.862328000	5.123573000
C	-1.967122000	10.322105000	7.692627000
C	-3.106424000	14.599790000	5.806418000
C	-3.705209000	15.677095000	7.873483000
N	-4.060567000	11.118124000	4.170320000
N	-1.737279000	11.165610000	3.954800000
C	-2.812468000	13.606649000	4.898181000
N	-2.500558000	9.078732000	7.774058000
N	-0.884728000	10.310338000	8.521712000
C	-3.078403000	15.913317000	5.045092000
C	-5.045430000	16.083189000	8.020556000
C	-2.649171000	16.399747000	8.461583000
Si	-2.989214000	10.455938000	2.947264000
C	-5.521538000	11.226868000	4.250339000
C	-0.285460000	11.016013000	4.002981000
C	-2.582613000	14.309473000	3.564724000
C	-1.785011000	8.293791000	8.662189000
C	-3.799098000	8.774095000	7.170788000
C	-0.761737000	9.072244000	9.133041000
C	0.041560000	11.445100000	8.673760000
H	-2.995693000	16.809375000	5.671020000
C	-4.306719000	15.914104000	4.094644000
C	-1.944162000	15.617069000	4.053883000
C	-5.309807000	17.236095000	8.763768000
C	-6.178759000	15.262741000	7.441470000
C	-2.962772000	17.550418000	9.190700000

C	-1.201526000	15.965666000	8.334056000
C	-3.107933000	11.191104000	1.227604000
C	-2.979394000	8.589618000	2.796369000
C	-6.126380000	9.916524000	4.765352000
C	-6.089136000	11.485807000	2.851584000
C	-5.936902000	12.360665000	5.185783000
C	0.355308000	12.238790000	4.661479000
C	0.082153000	9.737977000	4.766637000
C	0.227145000	10.905367000	2.566271000
C	-3.940998000	14.837374000	3.045569000
H	-2.012354000	13.717920000	2.836063000
C	-2.107502000	6.885507000	9.011738000
H	-3.916357000	9.571724000	6.422562000
C	-4.901220000	8.932886000	8.208394000
C	-3.825787000	7.442661000	6.437416000
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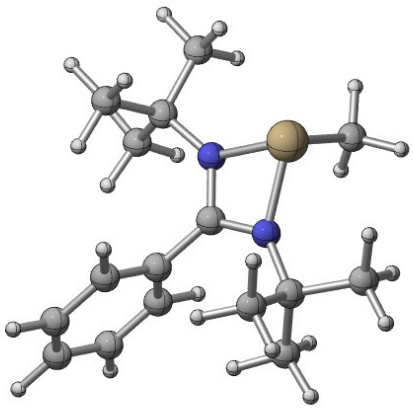
H	-0.442817000	12.225972000	8.066659000
C	0.125242000	11.951272000	10.104206000
C	1.406483000	11.151939000	8.065389000
H	-5.238293000	15.695606000	4.634823000
H	-4.425094000	16.906859000	3.634972000
H	-1.847895000	16.383967000	3.267789000
H	-0.973156000	15.462524000	4.547076000
H	-6.343197000	17.563187000	8.897391000
C	-4.279144000	17.968503000	9.342367000
H	-5.740873000	14.624205000	6.662148000
C	-7.262822000	16.112606000	6.785175000
C	-6.766310000	14.335982000	8.507205000
H	-2.158515000	18.124343000	9.657562000
H	-1.189316000	15.010071000	7.785371000
C	-0.381280000	16.970372000	7.524326000
C	-0.575196000	15.714201000	9.704923000
H	-3.211049000	12.284774000	1.274864000
H	-3.964858000	10.785910000	0.668222000
H	-2.198319000	10.956443000	0.652603000
H	-2.147897000	8.243931000	2.161543000
H	-3.913251000	8.236884000	2.329166000
H	-2.887864000	8.113909000	3.782178000
H	-5.768630000	9.061267000	4.171612000
H	-7.225309000	9.941040000	4.702370000
H	-5.857680000	9.751896000	5.815367000
H	-5.659545000	12.392768000	2.404607000
H	-7.182096000	11.606964000	2.895694000
H	-5.879772000	10.640453000	2.176301000
H	-5.508038000	12.220215000	6.189494000
H	-7.032566000	12.388293000	5.282707000
H	-5.599067000	13.333505000	4.807724000
H	0.124626000	13.149944000	4.090732000
H	1.448853000	12.121849000	4.704270000
H	-0.024395000	12.383581000	5.682932000
H	-0.319675000	9.770277000	5.788649000
H	1.173497000	9.600244000	4.824963000
H	-0.345906000	8.856432000	4.265223000
H	-0.204561000	10.029333000	2.055017000
H	1.321087000	10.787368000	2.552881000
H	-0.032187000	11.806026000	1.990180000
H	-4.685454000	14.035043000	2.973329000
H	-3.831237000	15.276122000	2.041077000

H	-1.467991000	6.556613000	9.839842000
H	-1.941397000	6.198165000	8.168601000
H	-3.150099000	6.768523000	9.340613000
H	-4.789211000	8.216914000	9.036023000
H	-5.885511000	8.759625000	7.749621000
H	-4.884599000	9.950964000	8.626500000
H	-2.911991000	7.300569000	5.842235000
H	-4.682512000	7.434324000	5.749251000
H	-3.940716000	6.583475000	7.111375000
H	0.235554000	7.632594000	10.334596000
H	0.071720000	9.219788000	11.108579000
H	1.281248000	8.967093000	9.832049000
H	-0.876887000	12.107307000	10.532211000
H	0.637023000	12.923892000	10.104922000
H	0.695360000	11.280657000	10.761506000
H	1.993497000	10.436949000	8.659998000
H	1.983024000	12.087467000	8.020210000
H	1.315414000	10.761924000	7.044118000
H	-4.504704000	18.866203000	9.922768000
H	-7.992564000	15.467516000	6.271123000
H	-6.840815000	16.809257000	6.044577000
H	-7.822938000	16.708139000	7.523101000
H	-5.987813000	13.699262000	8.955930000
H	-7.542414000	13.684284000	8.074598000
H	-7.222685000	14.917394000	9.324143000
H	-0.807035000	17.129672000	6.522788000
H	0.654055000	16.615026000	7.400228000
H	-0.338685000	17.949160000	8.028302000
H	0.453197000	15.334174000	9.594608000
H	-1.160865000	14.979260000	10.278325000
H	-0.521666000	16.638714000	10.300859000
Au	-3.387126000	13.060721000	10.306475000
Cl	-3.502679000	13.010180000	12.651939000



AMeSi

E = -1023.69100089

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N	26.17781500	8.05606900	9.66214500
C	26.29585600	6.73035700	9.59953000
C	25.30046700	5.72828600	10.06577000
C	25.32003300	5.27339800	11.38812300
C	24.33601000	5.23127100	9.18233400
H	26.07186400	5.65984500	12.07994200

C	24.38648400	4.33299800	11.82053500
C	23.40465500	4.29206700	9.61604900
H	24.32171400	5.58712800	8.14980700
H	24.40873100	3.98296100	12.85515000
C	23.42830700	3.84121300	10.93595300
H	22.65526500	3.90912900	8.91954000
H	22.69709500	3.10405200	11.27567700
C	27.82871200	8.79487100	7.38471800
H	27.66308800	9.88179300	7.29516900
H	28.76273400	8.57664200	6.83988900
H	26.99856900	8.26998500	6.88435000
C	28.24637100	5.22989700	8.93638100
C	28.71478600	4.69383200	10.29375600
C	27.41676900	4.17118100	8.20660800
C	29.46564300	5.58134600	8.08231800
H	29.28972700	5.46531600	10.82762900
H	27.85805100	4.40172300	10.91813600
H	29.35498600	3.80761500	10.16254600
H	27.00931800	4.57886700	7.26912200
H	28.05322700	3.30828000	7.95832700
H	26.58205000	3.80559800	8.81928700
H	30.11440100	4.70290200	7.95222000
H	29.15466300	5.93716300	7.08894200
H	30.05779700	6.37605600	8.56473500
C	25.14310700	8.91486300	10.22693300
C	23.74835600	8.53564600	9.72431200
C	25.18666200	8.86567000	11.75818300
C	25.47264900	10.33219200	9.75561800
H	23.73418900	8.48836200	8.62492000
H	23.41663400	7.56621600	10.11922800
H	23.01945600	9.29525000	10.04529600
H	26.19675900	9.11495500	12.11642500
H	24.47387100	9.58449000	12.19140200
H	24.92214200	7.86409300	12.12709300
H	24.76934800	11.05835300	10.18867200
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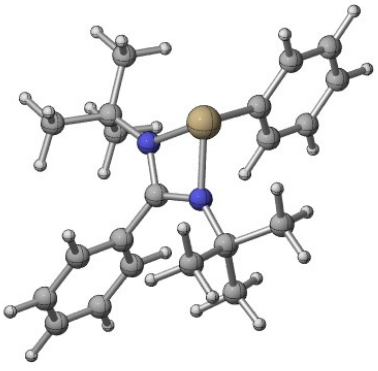
H	25.41515900	10.40027200	8.65914300



APhSi

E = -1215.27958758

Si	27.65783200	8.52431400	9.19392100
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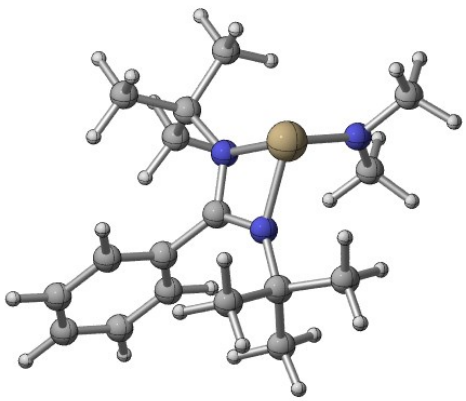
N	25.86606200	7.98474500	9.56227400
C	26.21606500	6.70513600	9.66437500
C	25.38224000	5.59447800	10.19595400
C	25.36731200	5.32381200	11.56841700
C	24.61244600	4.80852700	9.33208400
H	25.96190700	5.94173800	12.24503700
C	24.59467800	4.27798900	12.06859300

C	23.83900500	3.76501200	9.83449600
H	24.62808700	5.01560900	8.25971900
H	24.58915500	4.07295200	13.14158000
C	23.82970700	3.49749500	11.20294400
H	23.24142400	3.15585700	9.15256100
H	23.22368400	2.67801200	11.59615800
C	27.48452200	8.74437900	7.28474700
C	28.07709200	9.86139500	6.68026500
C	26.77755700	7.85628100	6.45823400
C	27.96569400	10.09260800	5.30703000
H	28.63899800	10.56860600	7.30034800
C	26.66270300	8.07419500	5.08794300
H	26.30977300	6.97044000	6.90131100
C	27.25766400	9.19792400	4.50861800
H	28.43515800	10.97271400	4.85940700
H	26.10828300	7.36790300	4.46353200
H	27.16905900	9.37212900	3.43310600
C	28.46326900	5.54197500	9.32269800
C	28.89570600	5.26785700	10.76667900
C	27.91374300	4.26620000	8.68098300
C	29.66487600	6.02934100	8.51132700
H	29.26731000	6.19246300	11.23351200
H	28.05475600	4.88750800	11.36470300
H	29.69870100	4.51510000	10.79555900
H	27.53315600	4.47668000	7.67002400
H	28.71718000	3.51901300	8.59578200
H	27.10409200	3.82074800	9.27429900
H	30.47089900	5.28129800	8.52536900
H	29.37684500	6.22020800	7.46704900
H	30.06064300	6.96746100	8.93322300
C	24.59457700	8.67110400	9.76407600
C	23.52932900	8.11109800	8.81691900
C	24.12760300	8.56493800	11.21871000
C	24.84675600	10.13918100	9.41811500
H	23.88722700	8.15129200	7.77724600
H	23.27842400	7.07010100	9.06438900
H	22.60558600	8.70522500	8.88966400
H	24.91369300	8.92646900	11.89876200
H	23.22643000	9.17752200	11.37528000
H	23.88100000	7.52861900	11.48895400
H	23.92812700	10.72855300	9.55236900
H	25.62818600	10.56248300	10.06825500
H	25.17619100	10.24077800	8.37297500

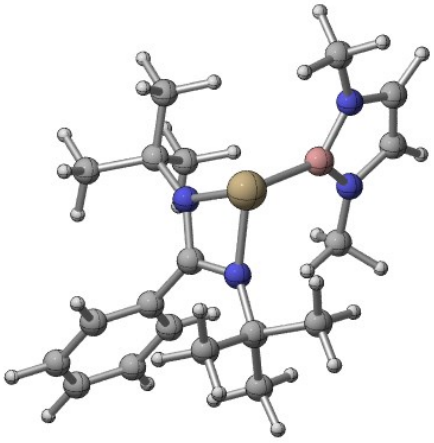


A(NMe$_2$)Si

E = -1118.30077822

Si	28.31282800	7.97150200	9.19350400
N	27.41592800	6.28766300	8.90376400

N	26.46501600	8.00512400	9.74907100
C	26.34097900	6.69105500	9.57699900
C	25.26309900	5.82443100	10.12477300
C	25.39022100	5.26383100	11.40003000
C	24.11435900	5.56219700	9.37065500
H	26.28639000	5.46728700	11.99053800
C	24.38075400	4.45183600	11.91306400
C	23.10694400	4.75027500	9.88535600
H	24.01462500	5.99966100	8.37480800
H	24.48836600	4.01824500	12.90998600
C	23.23822700	4.19372700	11.15726800
H	22.21355000	4.55092000	9.28918900
H	22.44749900	3.55686000	11.56046600
N	28.22151600	8.70611800	7.59887000
C	27.13402700	8.56149400	6.67396300
H	27.45916400	8.10411200	5.71670300
H	26.34777900	7.92045500	7.09885000
H	26.67052900	9.53723400	6.42030900
C	29.29279900	9.53471000	7.11786200
H	29.74761400	9.13557100	6.18808500
H	28.95644800	10.56769300	6.89319700
H	30.08876300	9.60087900	7.87655400
C	27.87292700	4.96346000	8.49833800
C	28.29609800	4.13066000	9.71290200
C	26.79678700	4.22713300	7.69695200
C	29.08791800	5.19922300	7.59857000
H	29.04133800	4.68061400	10.30714700
H	27.43537900	3.90001100	10.35690400
H	28.74213300	3.17657700	9.39166100
H	26.44952400	4.85023200	6.85874800
H	27.20960100	3.29411700	7.28411300
H	25.93070200	3.96363700	8.31896300
H	29.50203100	4.24111200	7.25170200
H	28.81011600	5.80373200	6.72276900
H	29.87624000	5.73888300	8.14629200
C	25.65296600	8.97438300	10.47570400
C	24.19401700	8.93134200	10.01505800
C	25.74093000	8.74365900	11.98790400
C	26.24011900	10.34644600	10.13815800
H	24.13439900	9.03482500	8.92091500
H	23.69991600	7.99428900	10.30526800
H	23.63259000	9.76138300	10.47026200
H	26.79356500	8.73634100	12.30862100
H	25.21630900	9.54382000	12.53282400
H	25.28149800	7.78594400	12.27156000
H	25.68476100	11.14139800	10.65718800
H	27.29535400	10.40246300	10.44804000
H	26.19534800	10.53145200	9.05492300



A(NHB)Si

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Si	27.72301400	8.98657500	9.28183400
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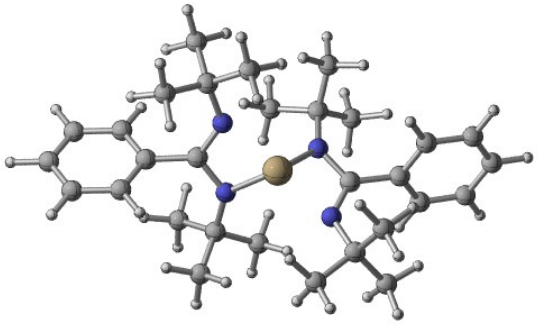
C	26.47607200	6.97508600	9.53006700
C	25.71098900	5.74901000	9.87053000
C	25.36053500	5.48009400	11.19835500
C	25.33247200	4.85138300	8.86625700
H	25.64507000	6.18670500	11.98120400
C	24.64777000	4.32663700	11.51670200
C	24.61465600	3.70116400	9.18552800
H	25.61112700	5.05740500	7.83042700
H	24.38044200	4.12325100	12.55627800
C	24.27314700	3.43595400	10.51110600
H	24.32236400	3.00650000	8.39469200
H	23.71233300	2.53242500	10.76148000
C	27.78249300	9.24091600	4.95915800
C	27.96572500	10.53943000	5.31725200
H	27.71874500	8.81518600	3.95843600
H	28.08042200	11.41143600	4.67477900
C	28.18171900	11.88213400	7.37655100
H	29.09748900	12.39515600	7.03843000
H	27.32891800	12.56321400	7.21191800
H	28.27006500	11.69884700	8.45694800
C	27.47434400	7.04362700	6.03239000
H	26.46153300	6.79936500	5.66495200
H	28.20277900	6.55620800	5.36270500
H	27.59197300	6.62121500	7.03759800
B	27.82172700	9.31007400	7.26105700
N	28.00196900	10.62683800	6.69687500
N	27.69230700	8.46207400	6.09951400
C	24.63268800	8.67537800	9.09947500
C	24.71359200	10.20208200	9.07617700
C	24.16747000	8.17257100	7.72872600
C	23.64942500	8.23994300	10.18896800
H	25.05977800	10.58844100	10.04625300
H	25.41824400	10.53671900	8.29825500
H	23.72774600	10.63656500	8.85532800
H	24.09015600	7.07532800	7.71931500
H	23.17680500	8.58335500	7.47982200
H	24.88151200	8.48266100	6.95105800
H	22.67460300	8.72487900	10.02716600
H	23.48826200	7.15350100	10.18667600
H	24.02039500	8.53500000	11.18206800
C	28.88498600	6.19308500	9.80716100
C	28.99707700	6.19131700	11.33531200

C	28.69732100	4.76414000	9.29281400
C	30.15891400	6.78139900	9.19925200
H	29.10909000	7.22123400	11.70621700
H	28.09781500	5.75194400	11.79207500
H	29.86650000	5.60073500	11.66376800
H	28.54373100	4.75505200	8.20308300
H	29.59966300	4.17380500	9.51289800
H	27.84446100	4.26113200	9.76737100
H	31.04228000	6.20302800	9.50715900
H	30.10259700	6.78080800	8.10041000
H	30.29598400	7.82272900	9.53432000

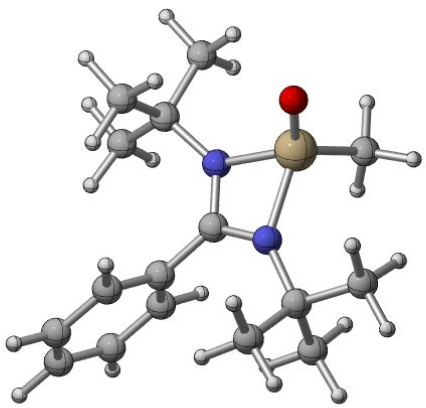


Tacke's bis(amidinato)silylene

E = -1678.23926798

C	-0.45575900	1.88833200	1.80675900
C	-1.29671000	-2.23855800	-0.85837100
C	-3.47572200	0.90168700	0.13909800
C	-3.36873300	-0.87750700	1.76772700
C	-4.84738900	1.01169200	0.34989000
C	-4.73909300	-0.75960800	1.98643400
C	-1.26781000	-0.18501300	0.59416200
C	-2.72691600	-0.04567400	0.84517100
C	-5.48144600	0.18350000	1.27629100
C	-1.57580700	-3.46580200	0.01710600
C	-0.26959900	-2.61461200	-1.93213200
C	-0.92332400	3.15096600	1.07568300
C	-1.40784900	1.58951500	2.97114300
H	-2.97709700	1.53597000	-0.59676900
H	-2.78110900	-1.60649600	2.32996000
H	-5.42689000	1.74615100	-0.21450700
H	-5.23086200	-1.40711900	2.71614700
H	-2.33041700	-3.23945600	0.78387700
H	-0.08752700	-1.76711200	-2.60754400
H	-0.27751700	3.35530800	0.21149600
H	-1.16842300	0.61992200	3.43385200
H	-6.55728200	0.27291000	1.44434400
H	-0.65952500	-3.80146500	0.52428100
H	0.69602900	-2.88430600	-1.48264100
H	-1.95615300	3.03993000	0.71724300
H	-2.46366000	1.58165100	2.67521700
H	-1.95519500	-4.29847200	-0.59546700
H	-0.63175100	-3.47276600	-2.51849900
H	-0.89149900	4.02276300	1.74762300
H	-1.28497600	2.36975400	3.73728300
N	-0.34984700	0.76178200	0.86291500
N	-0.68696900	-1.18791300	-0.03728400
C	3.21008400	2.28476300	-0.96442600
C	2.34092500	-1.82511500	1.69076300

C	5.48266800	0.65639800	1.46630000
C	5.23503200	-0.99646600	-0.27554600
C	6.84300300	0.36947100	1.54360500
C	6.59831300	-1.27312600	-0.20820300
C	3.20442900	0.23592100	0.48058400
C	4.66706200	-0.02884500	0.56090300
C	7.40385500	-0.59447000	0.70594700
C	2.44498500	-3.12831600	0.89606200
C	1.06512700	-1.84627100	2.53876700
C	2.06110400	3.21344200	-1.36330700
C	4.30068100	3.13021700	-0.29935400
H	5.03812800	1.40471100	2.12587300
H	4.59606400	-1.52756400	-0.98502200
H	7.47018000	0.90094500	2.26318800
H	7.03415500	-2.02496700	-0.87045700
H	3.36325100	-3.14601400	0.29122300
H	0.99497300	-0.93782400	3.15424800
H	1.22326500	2.62706100	-1.77098700
H	5.22052700	2.55780600	-0.12480400
H	8.47186300	-0.81696500	0.76555800
H	1.58450200	-3.23423200	0.22299800
H	0.17823800	-1.90360400	1.89699200
H	1.70123100	3.77908600	-0.49130300
H	3.94751000	3.53017700	0.66360200
H	2.46199200	-3.99728000	1.57189000
H	1.07616300	-2.71781400	3.21091800
H	2.39258900	3.93439800	-2.12539800
H	4.55542600	3.98204900	-0.94894700
N	2.62759300	1.29792500	-0.04854000
N	2.26039700	-0.68223200	0.76437200
Si	0.93741900	0.08629900	-0.36879300
C	-2.58288200	-1.82325400	-1.58395800
H	-3.43789000	-1.70384800	-0.90664000
H	-2.43312300	-0.87767300	-2.12654900
H	-2.84845300	-2.59746500	-2.32035900
C	0.92736400	2.13882100	2.41215800
H	1.26670400	1.25859800	2.97795300
H	1.66999300	2.33431900	1.62925700
H	0.88381800	2.99654800	3.09994500
C	3.75973800	1.60939500	-2.22609500
H	4.61512400	0.95970900	-1.99191400
H	2.97280200	0.99913700	-2.69434600
H	4.10026300	2.36527400	-2.95137100
C	3.52124000	-1.73448400	2.66370800
H	4.49394100	-1.89714200	2.18436700
H	3.54249900	-0.75919800	3.17277500
H	3.39610200	-2.51152600	3.43264500



AMeSiO
E = -1098.95023378

N	27.56482100	6.49924200	9.29211900
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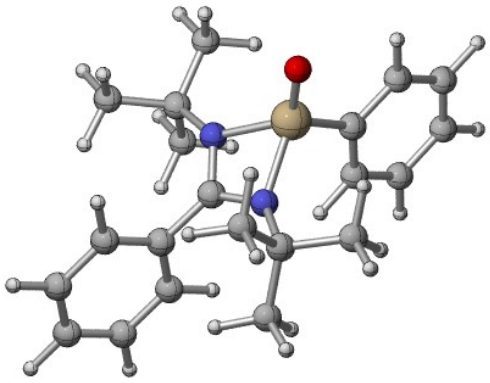
C	26.30584200	6.72990900	9.65571700
C	25.31300600	5.72094800	10.09937400
C	25.32152800	5.25551000	11.41762200
C	24.34214900	5.26017200	9.20477600
H	26.07997100	5.61903900	12.11418200
C	24.36123600	4.33744800	11.83687600
C	23.39092600	4.33490700	9.62568800
H	24.33239000	5.63558300	8.17917600
H	24.36741900	3.98115100	12.86937000
C	23.39726800	3.87484500	10.94223900
H	22.63613400	3.97521000	8.92285100
H	22.64659400	3.15331200	11.27263500
C	27.81150000	8.60157000	7.16452000
H	27.50541200	9.63785500	6.95243600
H	28.81749700	8.46846600	6.73787800
H	27.11416700	7.92025700	6.65390100
C	28.28618100	5.26155200	8.99834800
C	28.40927700	4.39024000	10.25072100
C	27.60126400	4.48515200	7.87091500
C	29.68331700	5.69618800	8.55276200
H	28.84552100	4.97028200	11.07738000
H	27.43436000	3.99818100	10.57064500
H	29.06570900	3.53094800	10.04656600
H	27.48612600	5.12061400	6.97960500
H	28.20383900	3.60780800	7.59080400
H	26.60757000	4.12685500	8.17632800
H	30.31832300	4.81789100	8.36760900
H	29.63330000	6.28097000	7.62186400
H	30.15780400	6.32146400	9.32399300
C	25.13504300	8.92283100	10.22928200
C	23.68826700	8.44936500	10.10262800
C	25.55293200	9.03341700	11.69955100
C	25.29154100	10.28630700	9.55386100
H	23.41820600	8.29186200	9.04736300
H	23.50502400	7.51548700	10.65080000
H	23.01721200	9.21680300	10.51669700
H	26.61346700	9.32239800	11.76019400
H	24.94199400	9.78501900	12.22276800
H	25.41941900	8.07014200	12.21559000
H	24.63321900	11.02817100	10.02868000
H	26.33153800	10.63725800	9.64734300
H	25.03186800	10.22371000	8.48597400
Si	27.84543600	8.33775600	9.01562000
O	28.75454200	9.14421900	9.97133800

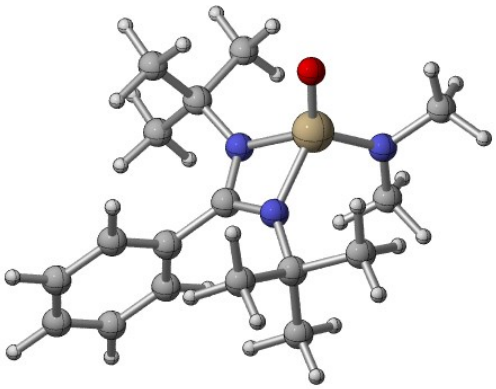


APhSIO

E = -1290.53764102

N	27.48440800	6.54263200	9.22864000
N	25.93563300	7.96947600	9.66242100
C	26.24393000	6.67627100	9.69940500
C	25.37391500	5.57097500	10.16807200
C	25.27178000	5.29221800	11.53418500
C	24.67701000	4.78757500	9.24311100
H	25.81622100	5.90765900	12.25355000
C	24.48011000	4.23189700	11.96953900
C	23.87982000	3.73488400	9.68395400
H	24.76636200	5.00271200	8.17608900
H	24.40702900	4.01381900	13.03727800
C	23.78269000	3.45394600	11.04651500
H	23.33485700	3.12701100	8.95839300
H	23.16070100	2.62439400	11.39032400
C	27.39745700	8.71479700	7.16221600
C	28.00681800	9.85720300	6.62466700
C	26.64441700	7.89485700	6.30883800
C	27.85586200	10.17952000	5.27601500
H	28.60722200	10.49039000	7.28449200
C	26.49288000	8.21062300	4.96048400
H	26.17707400	6.98656200	6.70244200
C	27.09726000	9.35785100	4.44368000
H	28.33511800	11.07454800	4.87104800
H	25.90520300	7.56068600	4.30688800
H	26.97931200	9.60816400	3.38625200
C	28.50268300	5.50752100	9.41336800
C	29.00614900	5.57018400	10.85893800
C	27.98381700	4.11148800	9.07426800
C	29.63721100	5.88250500	8.45833400
H	29.33190800	6.59461800	11.09497700
H	28.20947900	5.28279500	11.56232600
H	29.85265500	4.88214900	11.00630700
H	27.54656700	4.09118200	8.06449500
H	28.82030400	3.39718200	9.09843900
H	27.22624300	3.76271900	9.78898200
H	30.46905600	5.16947500	8.55204300
H	29.28631100	5.87768000	7.41536000
H	30.01574300	6.88968900	8.69413100
C	24.66720100	8.68399800	9.80985900
C	23.65291700	8.21092400	8.76571400
C	24.10672300	8.50972300	11.22273700
C	25.00014200	10.15802200	9.57346700
H	24.06916700	8.31351800	7.75237000
H	23.37008800	7.16062100	8.92813000

H	22.73687800	8.81799100	8.82457000
H	24.86012200	8.79666800	11.97132500
H	23.22404300	9.15295400	11.35669700
H	23.79773900	7.47264900	11.41293000
H	24.10366800	10.77973700	9.71036700
H	25.77821500	10.49631400	10.27406500
H	25.37243400	10.31414600	8.54920700
Si	27.63442400	8.37976100	8.98748400
O	28.66076200	9.19503700	9.80567800

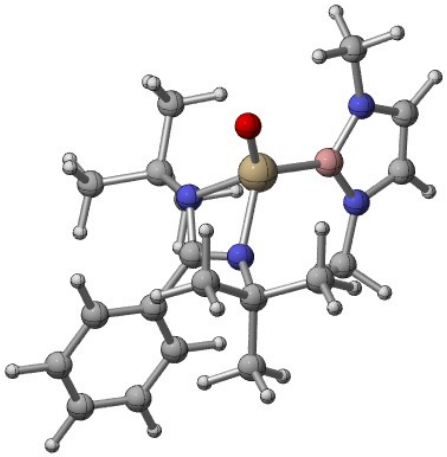


A(NMe$_2$)SiO

E = -1193.55745804

N	27.48555600	6.31574500	9.08322600
N	26.35794700	8.04590600	9.67957500
C	26.33960800	6.71258500	9.62667300
C	25.23252500	5.84342200	10.09011500
C	25.30962600	5.20370500	11.33072800
C	24.09489900	5.68225800	9.29272100
H	26.19781500	5.33473100	11.95234100
C	24.25149100	4.41119300	11.77049700
C	23.04522800	4.88058600	9.73203400
H	24.03565600	6.19074800	8.32796700
H	24.31250700	3.91871800	12.74349700
C	23.12078700	4.24653300	10.97203700
H	22.16031300	4.75415500	9.10439200
H	22.29381000	3.62219600	11.31781600
N	28.13025500	8.61893900	7.43167800
C	27.11266300	8.31572200	6.46852400
H	27.49038800	7.69036200	5.63331200
H	26.27845200	7.77428600	6.93978400
H	26.68892600	9.23454900	6.01734200
C	29.22435900	9.42691100	6.95625900
H	29.77772100	8.93275500	6.13295900
H	28.87468300	10.40704000	6.57659900
H	29.92475600	9.60701500	7.78468100
C	27.95546400	5.02056300	8.59452800
C	28.16223300	4.04748400	9.75774900
C	26.98210600	4.43411200	7.57005200
C	29.30184400	5.30485300	7.92618000
H	28.81063200	4.50105700	10.52190600
H	27.20741200	3.76838300	10.22468600
H	28.64255300	3.12509700	9.39765300
H	26.81442100	5.14420300	6.74626400
H	27.39492000	3.50701400	7.14454300
H	26.01209900	4.19082900	8.02685800
H	29.74842900	4.37365400	7.54893300
H	29.17762400	6.00254600	7.08473200
H	29.99650500	5.76432800	8.64619000

C	25.66717800	8.99117000	10.56095600
C	24.14890200	8.83970400	10.49726500
C	26.18299900	8.80118300	11.99107700
C	26.07202600	10.37716000	10.05569300
H	23.79366600	8.89760600	9.45706800
H	23.80690500	7.88967300	10.92967700
H	23.67654100	9.65471900	11.06586400
H	27.28265500	8.85494000	11.99417400
H	25.78098500	9.58062200	12.65636100
H	25.87416000	7.82323600	12.39129800
H	25.60505700	11.16110000	10.66945700
H	27.16567000	10.49350200	10.11561600
H	25.76117200	10.51684700	9.00941200
Si	28.11983100	8.07907700	9.06407100
O	29.22939900	8.53029400	10.04107600



A(NHB)SiO

E = -1350.49768020

N	27.78217500	7.04779200	9.38311100
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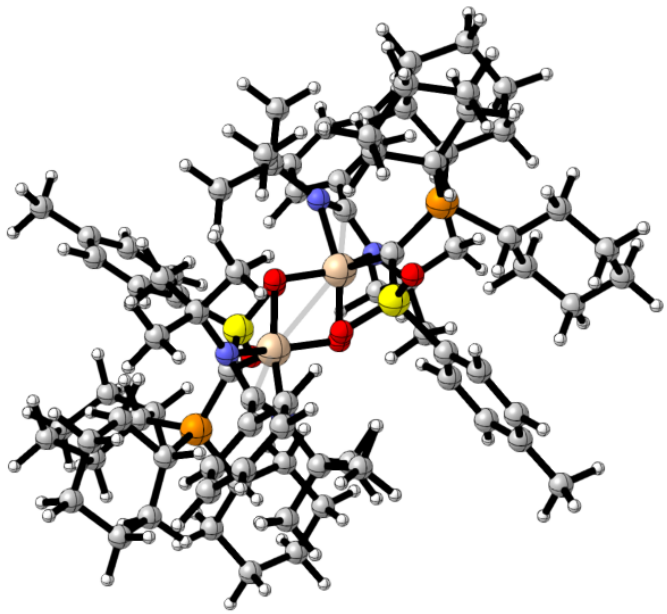
C	26.46237300	6.96709900	9.56351900
C	25.70629900	5.72316800	9.84988400
C	25.32230500	5.42378100	11.16053700
C	25.39610600	4.83655700	8.81442000
H	25.56151700	6.12221400	11.96532900
C	24.63829600	4.24138700	11.43190000
C	24.70304300	3.66040800	9.08899400
H	25.70436900	5.06972400	7.79300800
H	24.34482000	4.00867100	12.45795600
C	24.32650000	3.35972400	10.39750000
H	24.45986600	2.97202200	8.27654000
H	23.78766400	2.43404000	10.61211900
C	27.75042200	9.33288000	4.84434600
C	28.05369700	10.59279100	5.26041400
H	27.64980600	8.95860600	3.82656700
H	28.25272900	11.47623900	4.65533300
C	28.41875900	11.80287500	7.40354300
H	29.37464700	12.23699500	7.06862300
H	27.63675500	12.57395400	7.29991200
H	28.51093600	11.52205400	8.46441200
C	27.28355900	7.11534500	5.83773100
H	26.24498500	6.94151100	5.50459200
H	27.95680600	6.61671100	5.12136500
H	27.41977400	6.63771800	6.81755600
B	27.79711900	9.30714400	7.13244300
N	28.09633400	10.61987000	6.64061000
N	27.58912000	8.51508900	5.95093900

C	24.59716400	8.65810300	9.16290000
C	24.69295700	10.18483000	9.14264300
C	24.10946700	8.15493200	7.80108200
C	23.63570300	8.22493700	10.27058700
H	25.10869700	10.55928000	10.08936900
H	25.35264900	10.52190800	8.32747400
H	23.70003900	10.63031800	8.98474700
H	24.02541000	7.05790200	7.79120100
H	23.11742700	8.57162500	7.56919800
H	24.80829100	8.46437000	7.00927500
H	22.65902200	8.70979400	10.12300700
H	23.47365800	7.13860200	10.27352300
H	24.02337600	8.52519200	11.25547600
C	28.88806700	6.23271000	9.88704300
C	28.99579600	6.44454400	11.40086200
C	28.72535500	4.75181600	9.54921200
C	30.14127400	6.78471800	9.20559700
H	29.05597100	7.52203300	11.61794000
H	28.11514900	6.02991000	11.91547700
H	29.89013800	5.94388900	11.80268300
H	28.57714100	4.60973500	8.46764700
H	29.63607200	4.20830900	9.84247800
H	27.87809600	4.29421800	10.07766300
H	31.03549800	6.24453100	9.54900200
H	30.06917800	6.68152100	8.11187600
H	30.26452000	7.85200600	9.44819700
Si	27.68056500	8.89245700	9.07694300
O	28.33515100	9.83831300	10.12361400



6-Dimer

E = -5923.916346

P	11.961884000	8.632106000	17.047976000
C	12.603327000	10.127814000	17.739006000
Si	11.779374000	11.584247000	18.740196000
Si	13.397695000	13.014310000	20.170772000
O	12.711105000	13.024748000	18.592804000
O	12.435473000	11.563654000	20.347843000
N	9.974768000	10.943914000	19.130742000
N	10.383659000	12.413621000	17.604189000
C	9.429530000	11.866738000	18.332396000
C	12.589701000	14.300584000	21.361728000
N	15.026075000	13.909703000	19.488291000
N	15.014947000	12.419020000	21.055728000
C	15.786673000	13.100494000	20.206631000

C	9.285443000	10.113589000	20.133367000
C	10.347467000	13.632452000	16.771998000
C	7.991960000	12.260948000	18.312851000
P	13.180010000	15.572654000	22.438731000
C	15.330326000	14.632887000	18.234809000
C	15.436958000	11.365195000	21.998722000
C	17.255470000	12.916336000	20.031082000
C	10.370340000	9.402437000	20.932602000
C	8.406173000	10.935781000	21.084539000
C	8.397050000	9.051605000	19.473840000
C	10.428943000	14.894178000	17.639403000
C	9.100525000	13.732958000	15.887223000
C	11.567687000	13.582557000	15.850094000
C	7.568159000	13.355754000	19.076591000
C	7.065556000	11.578933000	17.521639000
C	14.225322000	15.673633000	18.042446000
C	15.298198000	13.693307000	17.027094000
C	16.687047000	15.347046000	18.238663000
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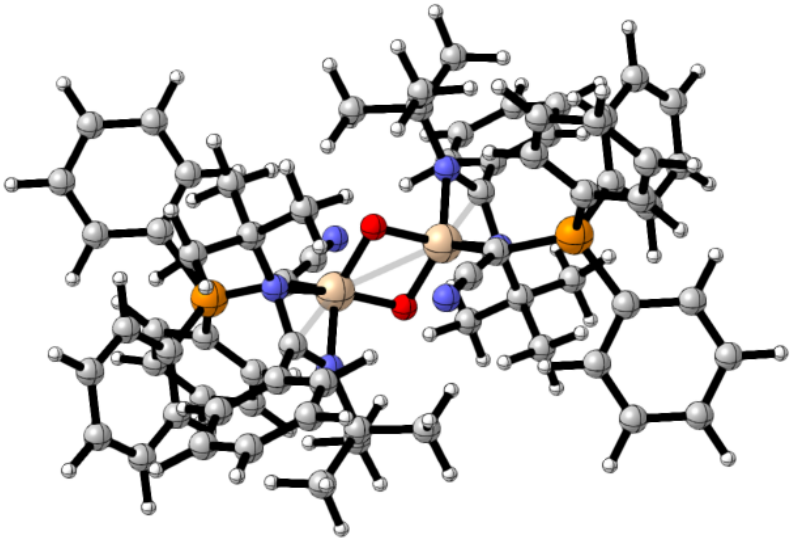

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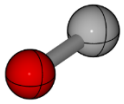
C	11.104368000	13.439676000	21.763251000
N	9.974465000	13.191562000	21.936499000



CO

E = -113.231244798

C	-4.51534200	2.57361600	0.00000000
O	-3.38727300	2.57361600	0.00000000

8. References

[22] H. Darmandeh, T. Scherpf, K.-S. Feichtner, C. Schwarz, V. H. Gessner, *Z. Anorg. Allg. Chem.* **2020**, *646*, 835 – 841.

[26b] S. S. Sen, H. W. Roesky, D. Stern, J. Henn, D. Stalke, *J. Am. Chem. Soc.* **2010**, *132*, 1123 – 1126.

[27a] T. Scherpf, R. Wirth, S. Molitor, K.-S. Feichtner, V. H. Gessner, *Angew. Chem. Int. Ed.* **2015**, *54*, 8542 – 8546.

[27b] C. Schwarz, L. T. Scharf, T. Scherpf, J. Weismann, V. H. Gessner, *Chem. Eur. J.* **2019**, *25*, 2793 – 2802.

[30] a) P. Hohenberg, W. Kohn, *Phys. Rev.* **1964**, *136*, B864 – B871. b) W. Kohn, L. J. Sham, *Phys Rev.* **1965**, *140*, A1133 – A1138.

[31] a) C. Adamo, V. Barone, *J. Chem. Phys.* **1999**, *110*, 6158 – 6169. b) A. Schaefer, H. Horn, R. Ahlrichs, *J. Chem. Phys.* **1992**, *97*, 2571 – 2577. c) A. Schaefer, C. Huber, R. Ahlrichs, *J. Chem. Phys.* **1994**, *100*, 5829 – 5835.

[36] G. M. Sheldrick, *Acta Cryst.* **2008**, *A64*, 112.

[37] G. M. Sheldrick, *Acta Cryst.* **2015**, *C71*, 3.

[38] A. Thorn, B. Dittrich, G. M. Sheldrick, *Acta Cryst.* **2012**, *A68*, 448.

[39] G. M. Sheldrick, *Acta Cryst.* **2015**, *A71*, 3.

[40] GaussView, Version 6.1, Roy Dennington, Todd A. Keith, and John M. Millam, Semichem Inc., Shawnee Mission, KS, 2016.

[41] Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[42] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297 – 3305.

[43] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.

[44] S. Grimme, S. Ehrlich, L. Goerigk, *J. Comp. Chem.* **2011**, *32*, 1456 – 1465.

[45] NBO 7.0. E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, P. Karafiloglou, C. R. Landis, and F. Weinhold, Theoretical Chemistry Institute, University of Wisconsin, Madison, WI (2018).

[46] R. F. W. Bader, *Chem. Rev.* **1991**, *91*, 893 – 928.

[47] E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen, W. Yang, *J. Am. Chem. Soc.* **2010**, *132*, 6498 – 6506.

[48] T. Lu, F. Chen, *J. Comput. Chem.* **2012**, *33*, 580 – 592.

[49] W. Humphrey, A. Dalke, K. Schulten, *J. Molec. Graphics* **1996**, *14*, 33 – 38.