

Supporting Information

Hydrosilylation Catalysis by Earth Alkaline Metal Silyl: Synthesis, Characterization, and Reactivity of Bis(triphenylsilyl)calcium

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General Experimental Remarks.

All operations were performed under an inert atmosphere of dry argon using standard Schlenk line or glove box techniques. d_8 -THF and C_6D_6 were distilled under argon from sodium/benzophenone ketyl prior to use. 1,1-Diphenylethene, phenylsilane, diphenylsilane and d_5 -pyridine were dried over CaH_2 and distilled under argon prior to use. Triphenylsilane was purified by vacuum sublimation. THF and pentane were purified using a MB SPS-800 solvent purification system. Triphenylsilyl potassium **1** was prepared according to literature.¹

Due to extreme sensitivity, elemental analysis by combustion could not be performed. Instead, metal titration by following the procedure was applied: 20-30 mg of the product were dissolved in 1 mL of THF and hydrolyzed. To this solution 1 mL of an aqueous ammonia solution (25%) and a buffer tablet (Eriochrome black T) were added and the mixture titrated with a 0.01 M solution of EDTA disodium salt until the transition from red to green was observed.

NMR spectra were recorded on a Bruker Avance II 400 spectrometer at 25 °C unless otherwise stated. Chemical shifts for 1H , $^{13}C\{^1H\}$ and $^{29}Si\{^1H\}$ NMR spectra were referenced internally using the residual solvent resonance and are reported relative to tetramethylsilane. The resonances in 1H and ^{13}C NMR spectra were assigned on the basis of two-dimensional NMR experiments (COSY, HSQC, HMBC).

Experimental Section

Preparation of [Ca(SiPh₃)₂(thf)₄] (2a**).** A solution of [KSiPh₃(thf)₁] (**1**) (556 mg, 1.5 mmol) in THF (5 mL) was added to a suspension of anhydrous CaI₂ (220 mg, 0.75 mmol) in THF (5 mL). The colorless precipitate was filtered off and the solvent was removed under reduced pressure. After washing with pentane (3 × 2 mL) and subsequent drying, [Ca(SiPh₃)₂(thf)₄] (**2a**) (635 mg, 0.75 mmol, >99%) was obtained as a pale yellow powder. Yellow crystals of [Ca(SiPh₃)₂(thf)₄] (**2a**) (491 mg, 0.58 mmol, 77%) suitable for single crystal X-ray analysis were grown from THF/pentane within 1 h at -30 °C.

1H NMR (d_8 -THF, 400.1 MHz): δ 1.77 (m, 16H, thf), 3.62 (m, 16H, thf), 6.94-6.97 (m, 6H, *para*-Ph), 7.01-7.04 (m, 12H, *meta*-Ph), 7.37-7.39 (m, 12H, *ortho*-Ph). $^{13}C\{^1H\}$ NMR (d_8 -THF, 100.6 MHz): δ 26.39 (thf), 68.21 (thf), 125.46 (*para*-Ph), 127.27 (*meta*-Ph), 137.12 (*ortho*-Ph), 144.97 (*ipso*-Ph). $^{29}Si\{^1H\}$ NMR (d_8 -THF, 25 °C, 79.5 MHz): δ -13.99 (CaSi). 1H NMR (C_6D_6 , 400.1 MHz): δ 1.21 (m, 16H, thf), 3.52 (m, 16H, thf), 7.16-7.20 (m, 6H, *para*-Ph), 7.26-7.30 (m, 12H, *meta*-Ph), 7.77-7.79 (m, 12H, *ortho*-Ph). $^{13}C\{^1H\}$ NMR (C_6D_6 ,

100.6 MHz): δ 25.86 (thf), 69.13 (thf), 126.12 (*para*-Ph), 127.75 (*meta*-Ph), 137.07 (*ortho*-Ph), 152.93 (*ipso*-Ph). $^{29}\text{Si}\{\text{H}\}$ NMR (C_6D_6 , 79.5 MHz): δ -12.99 (CaSi). Anal. calc. for $\text{C}_{52}\text{H}_{62}\text{CaO}_4\text{Si}_2$ (847.30 g mol⁻¹): Ca, 4.73. Found: Ca, 4.53%.

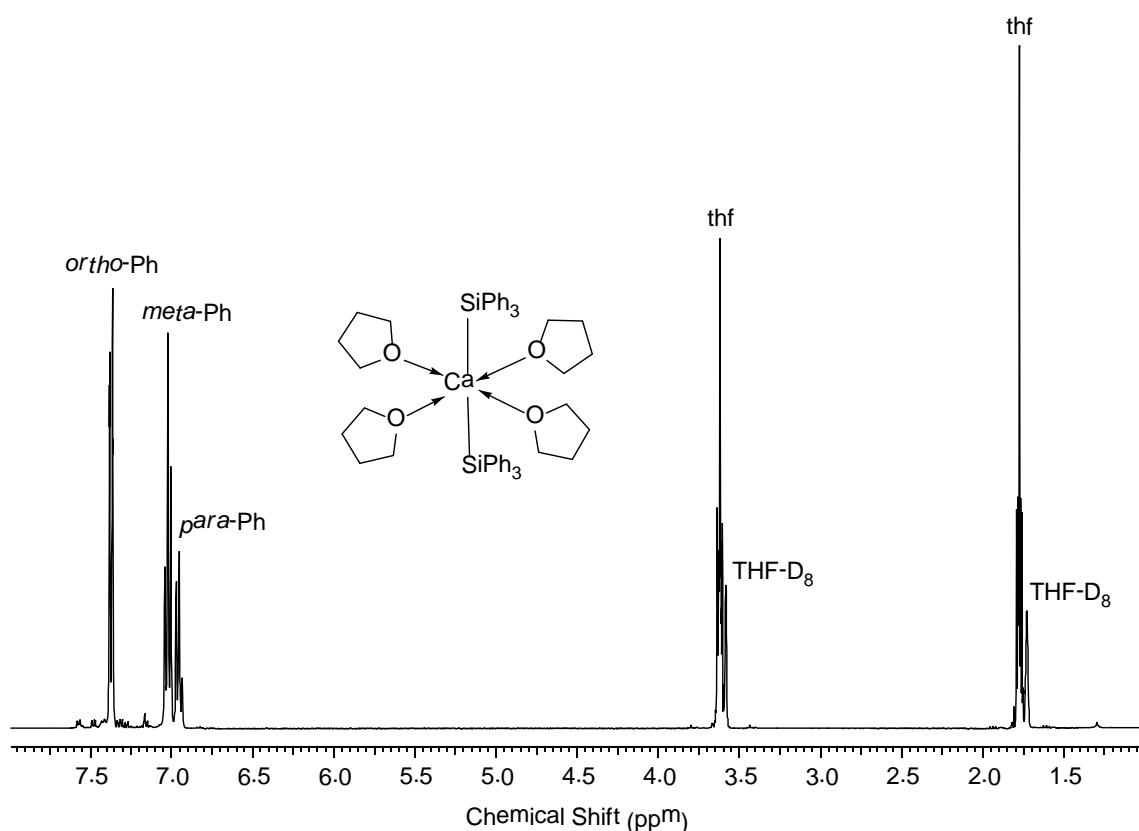


Figure S1 ^1H NMR spectrum of **2a** in $\text{d}_8\text{-THF}$ at 25 °C.

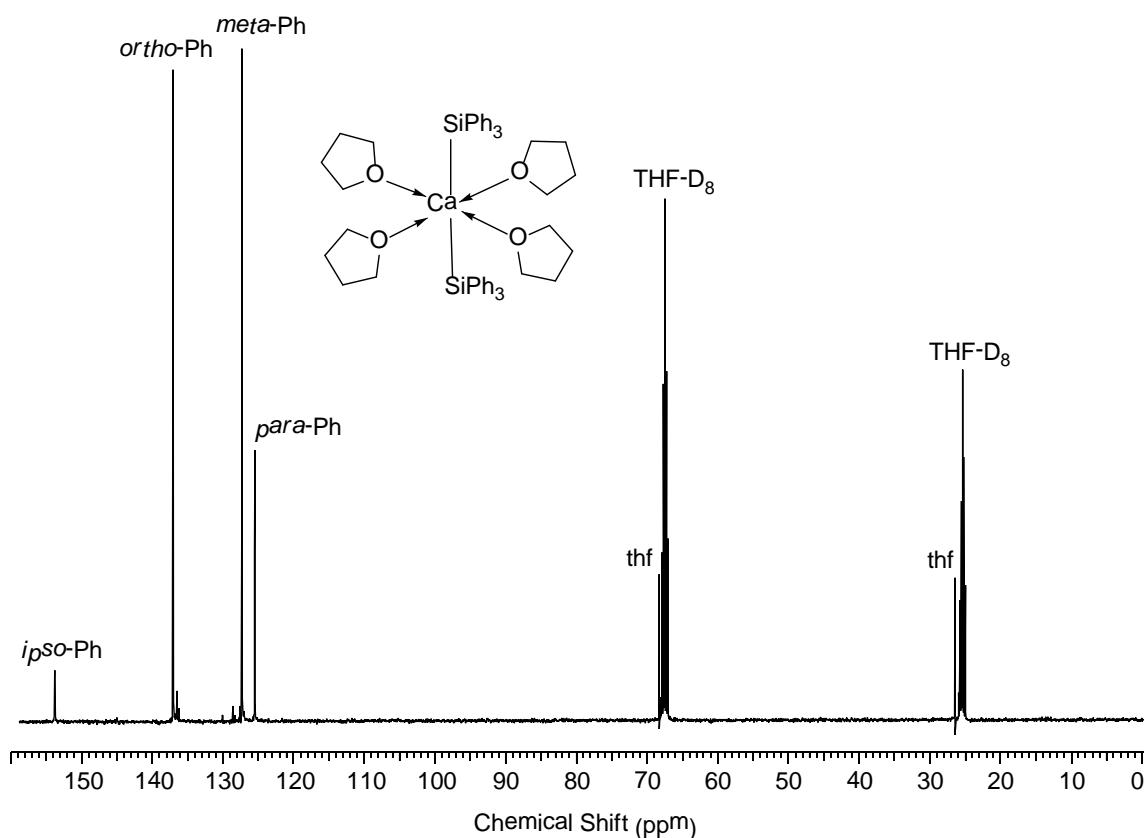


Figure S2 $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **2a** in $\text{d}_8\text{-THF}$ at 25°C .

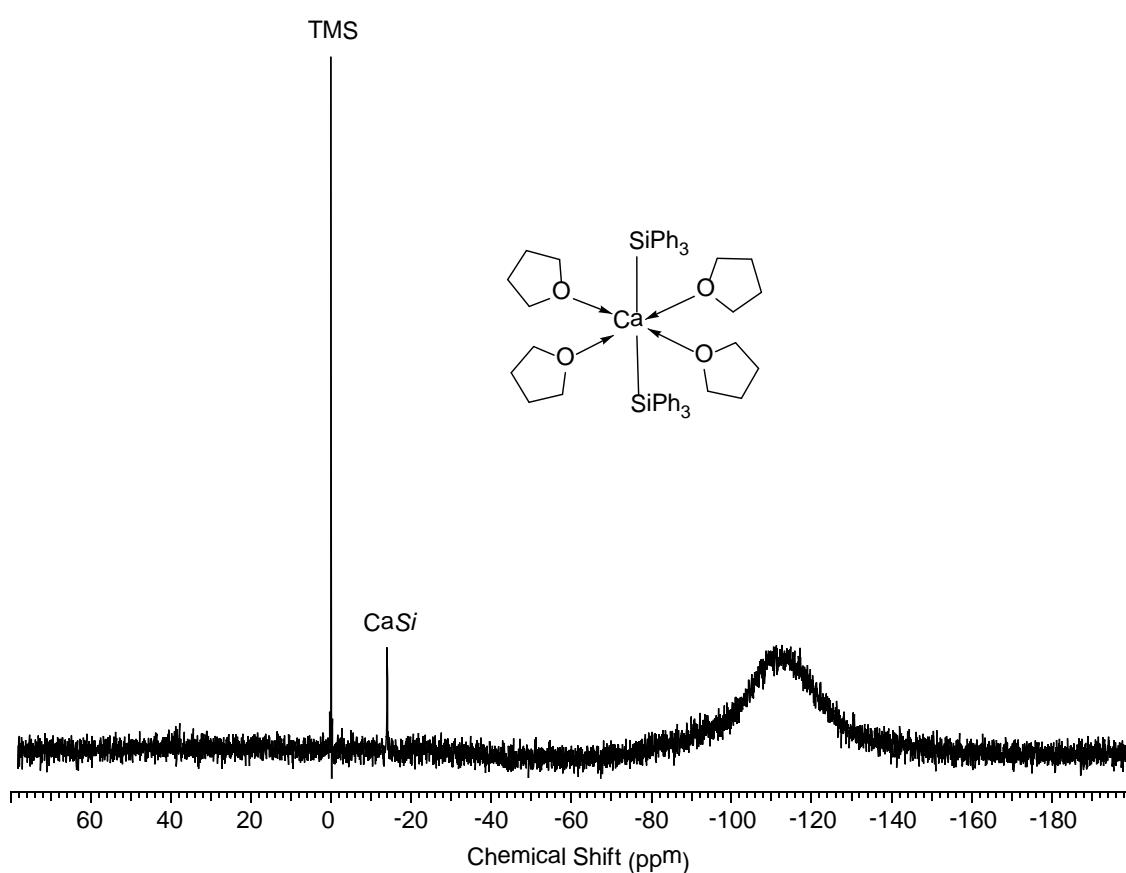


Figure S3 $^{29}\text{Si}\{\text{H}\}$ NMR spectrum of **2a** in $\text{d}_8\text{-THF}$ at 25°C .

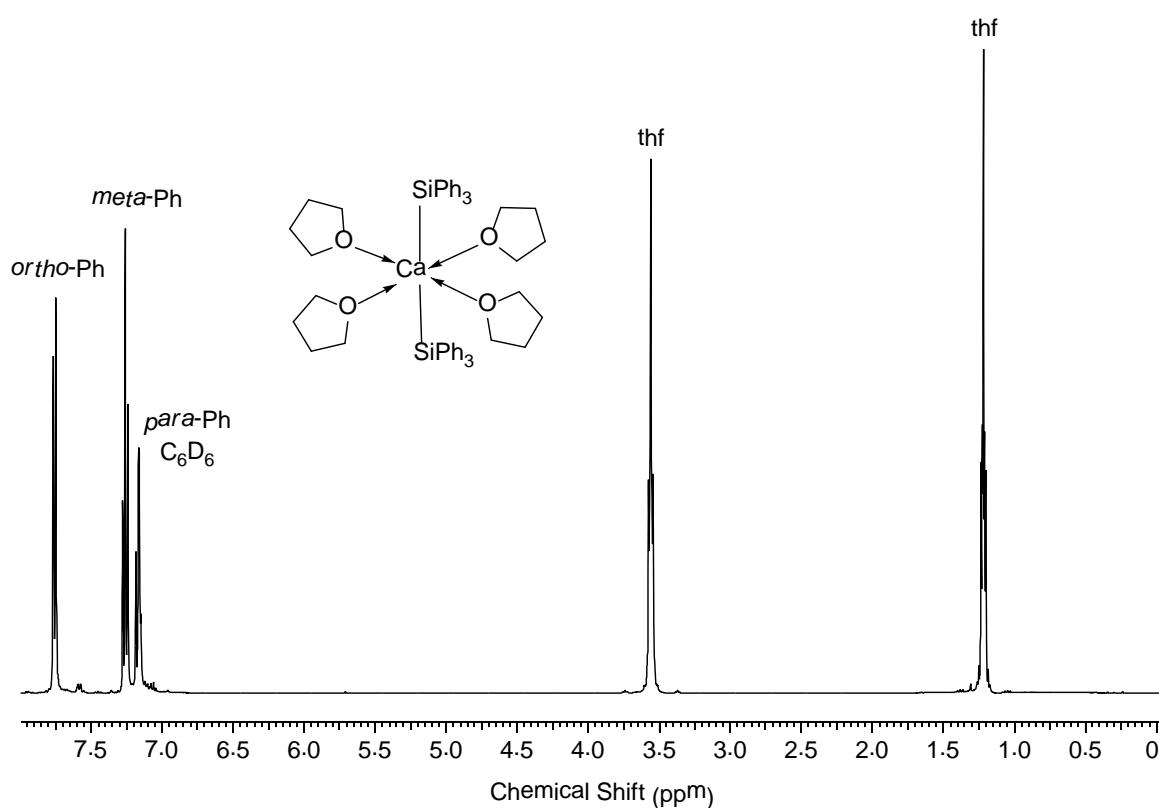


Figure S4 ^1H NMR spectrum of **2a** in C_6D_6 at 25°C .

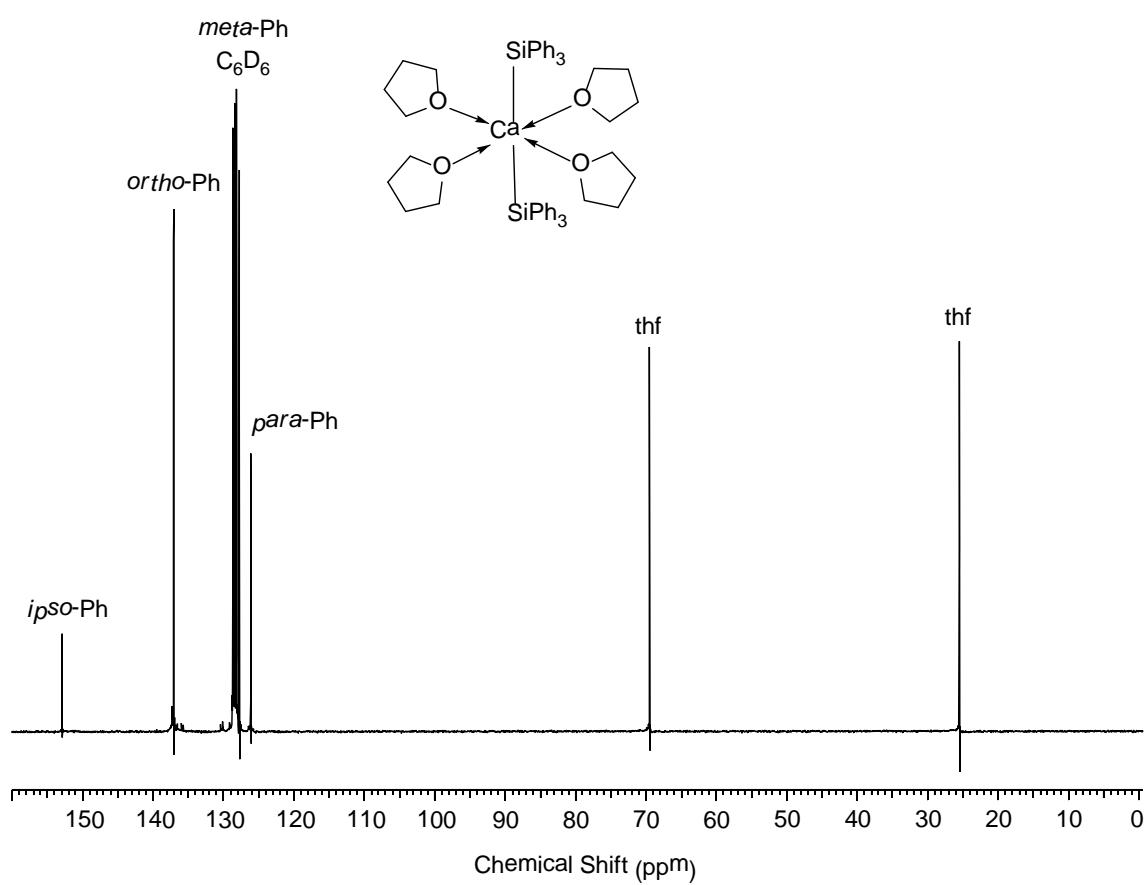


Figure S5 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2a** in C_6D_6 at 25°C .

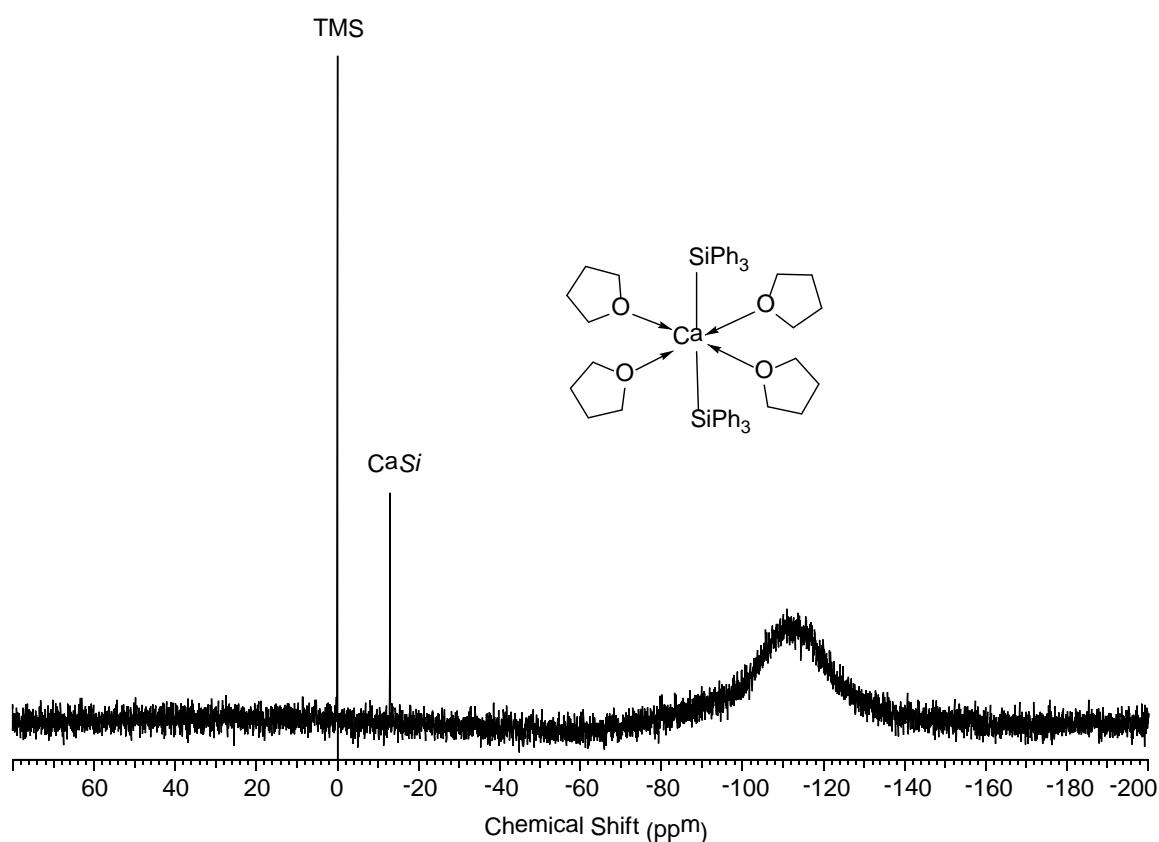


Figure S6 $^{29}\text{Si}\{\text{H}\}$ NMR spectrum of **2a** in C₆D₆ at 25 °C.

Preparation of [Ca(SiPh₃)₂(triglyme-κ⁴)(thf)] (2b). To a solution of [Ca(SiPh₃)₂(thf)₄] (2a) (170 mg, 0.2 mmol) in THF (1 mL) was added a solution of triglyme (36 mg, 0.2 mmol) in pentane (0.5 mL). Orange crystals suitable for single X-ray analysis formed within 1 h at –30 °C. The mother liquor was decanted off and the pale orange crystals of [Ca(SiPh₃)₂(triglyme-κ⁴)(thf)] (2b) (130 mg, 80%) were isolated.

¹H NMR (d₈-THF, 400.1 MHz): δ 1.78 (m, 4H, thf), 3.33 (br s, 12H, CH₂), 3.50-3.52 (m, 6H, CH₃), 3.62 (m, 4H, thf), 6.93-6.96 (m, 6H, *para*-Ph), 7.01-7.05 (m, 12H, *meta*-Ph), 7.39-7.42 (m, 12H, *ortho*-Ph). ¹³C{¹H} NMR (d₈-THF, 100.6 MHz): δ 26.44 (thf), 60.15 (CH₂), 68.28 (thf), 70.23 (CH₃/CH₂), 70.48 (CH₃/CH₂), 72.61 (CH₃), 125.31 (*para*-Ph), 127.22 (*meta*-Ph), 137.14 (*ortho*-Ph), 154.14 (*ipso*-Ph). ²⁹Si{¹H} NMR (d₈-THF, 79.5 MHz): δ –11.19 (CaSi). ¹H NMR (C₆D₆, 400.1 MHz): δ 1.31 (m, 4H, thf), 2.65 (br s, 3H, CH₃), 2.82 (br s, 3H, CH₃), 2.96 (br s, 12H, CH₂), 3.58 (m, 4H, thf), 7.14-7.18 (m, 6H, *para*-Ph), 7.23-7.27 (m, 12H, *meta*-Ph), 7.71-7.74 (m, 12H, *ortho*-Ph). ¹³C{¹H} NMR (C₆D₆, 100.6 MHz): δ 25.88 (thf), 60.03 (CH₂), 68.70 (thf), 69.26 (CH₃), 69.38 (CH₃), 71.20 (CH₂), 125.86 (*para*-Ph), 127.62 (*meta*-Ph), 137.11 (*ortho*-Ph), 153.39 (*ipso*-Ph). ²⁹Si{¹H} NMR (C₆D₆, 79.5 MHz): δ –13.70 (CaSi). Anal. calc. for C₄₈H₅₆CaO₅Si₂ (809.20 g mol^{–1}): Ca, 4.95. Found: Ca, 4.28%.

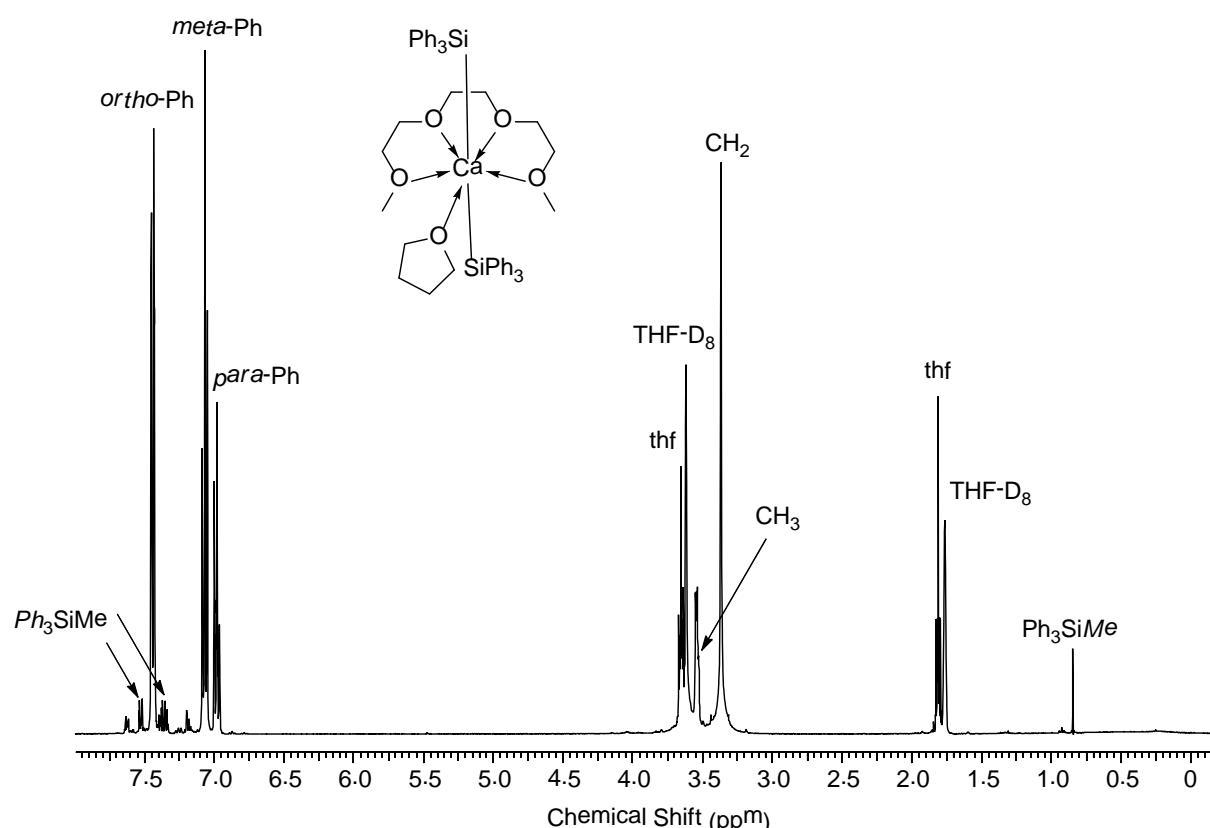


Figure S7 ^1H NMR spectrum of **2b** in $\text{d}_8\text{-THF}$ at $25\text{ }^\circ\text{C}$.

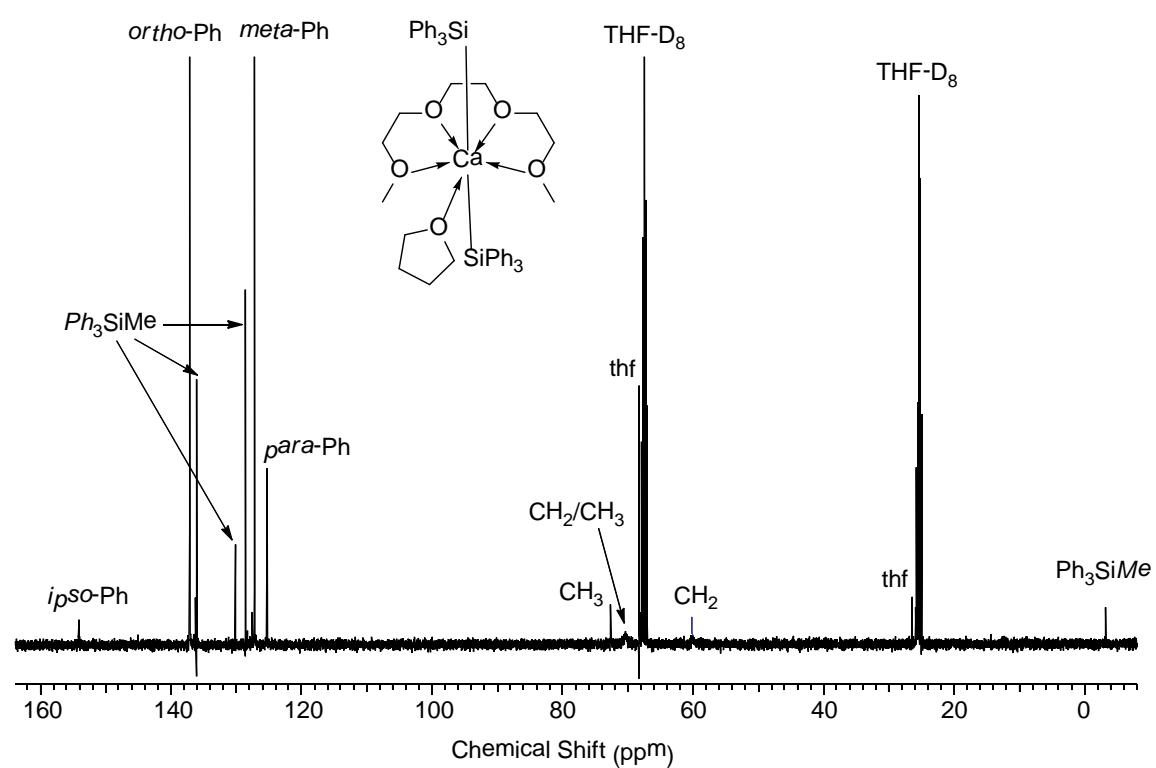


Figure S8 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2b** in $\text{d}_8\text{-THF}$ at $25\text{ }^\circ\text{C}$.

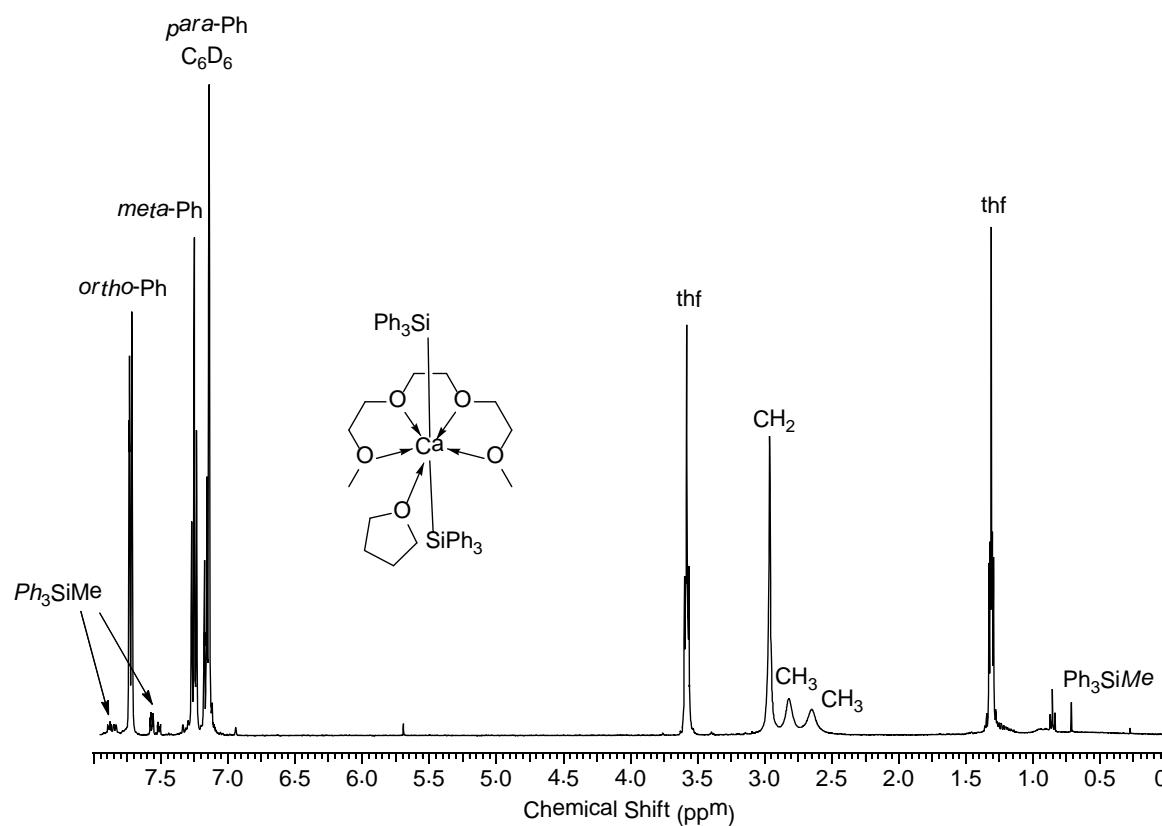


Figure S9 ^1H NMR spectrum of **2b** in C_6D_6 at 25°C .

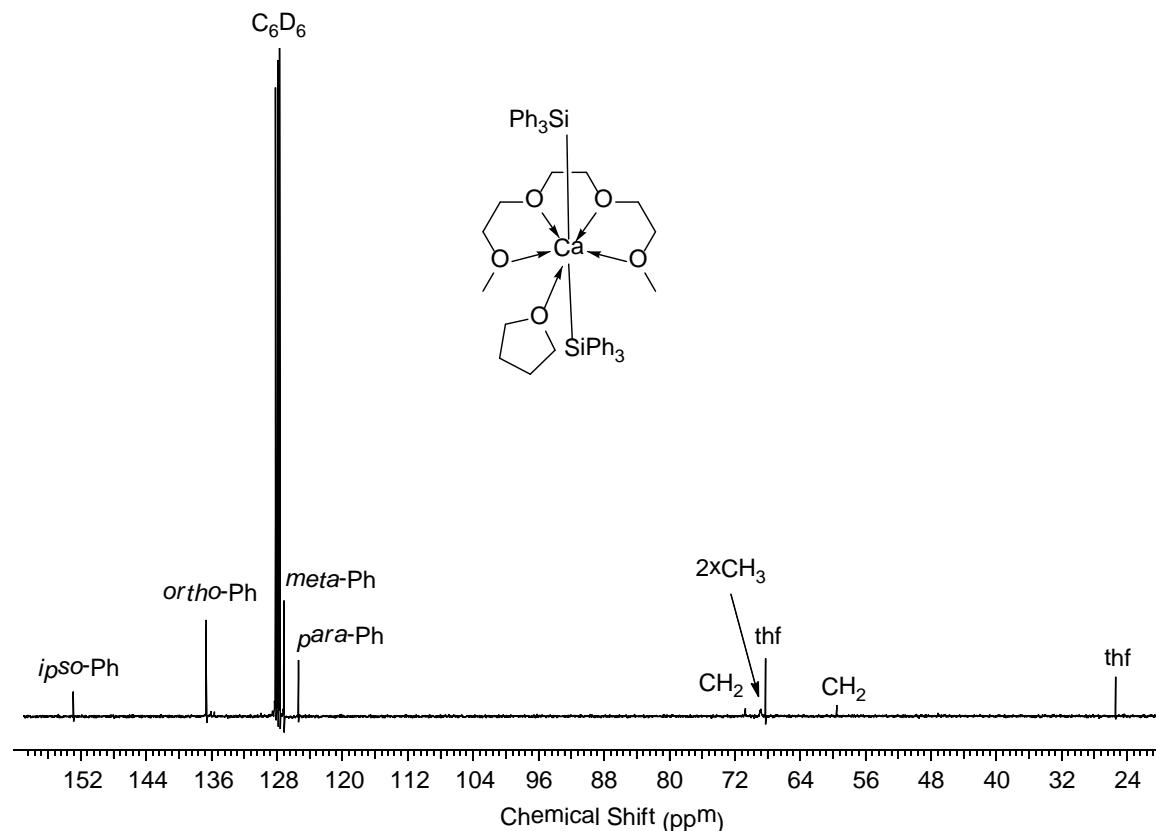


Figure S10 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2b** in C_6D_6 at 25°C .

Reaction of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (2a**) with H_2O .** Water (0.9 μL , 0.05 mmol) was added to a solution of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (**2a**) (21 mg, 0.025 mmol) in C_6D_6 (0.5 mL). The pale yellow solution decolorized and triphenylsilane was detected as the only product by ^1H NMR spectroscopy. Upon addition of water (0.5 mL) to the reaction mixture a pH value of 12 was observed, which indicates the formation of calcium hydroxide.

Triphenylsilane²

^1H NMR (C_6D_6 , 400.1 MHz): δ 5.71 (s, 1H, Ph_3SiH), 7.12-7.19 (m, 9H, *para/meta*-Ph), 7.58-7.60 (m, 6H, *ortho*-Ph).

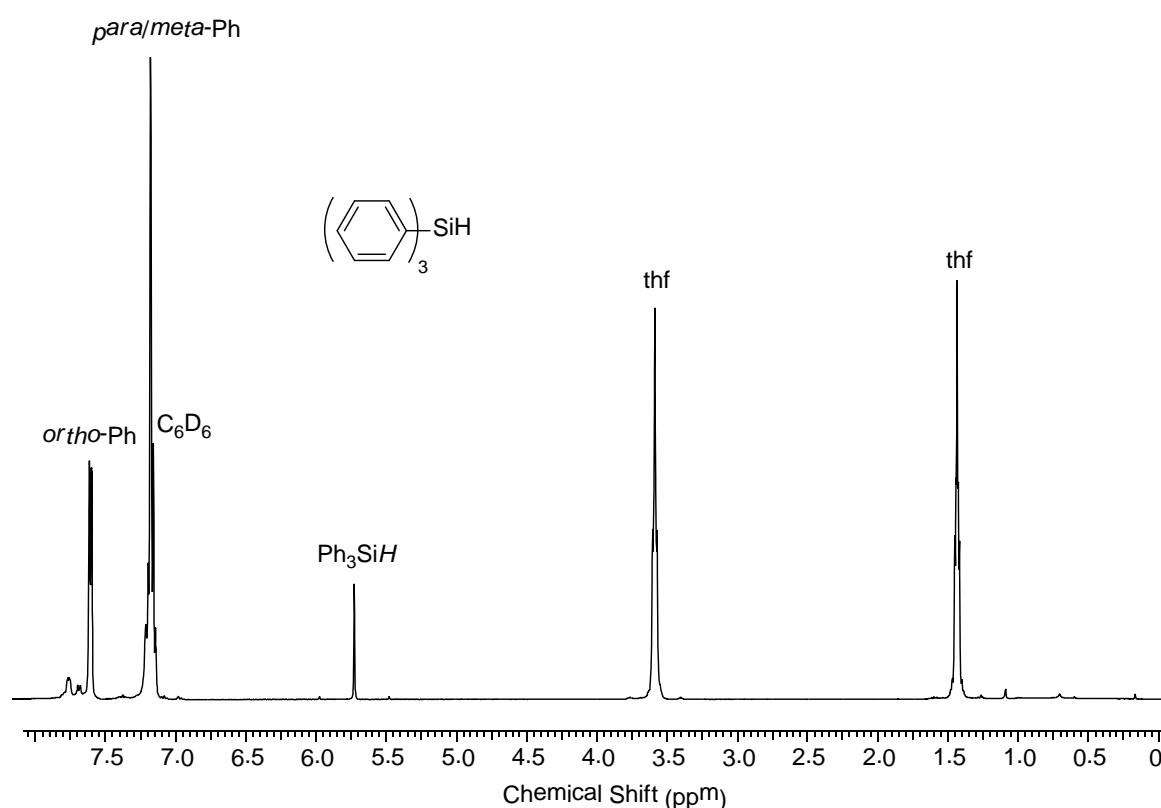


Figure S11 ^1H NMR spectrum of **2a** in C_6D_6 at 25 °C after reaction with H_2O .

Reaction of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (2a**) with Me_3SiCl .** Chlorotrimethylsilane (6.5 μL , 0.05 mmol) was added to a solution of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (**2a**) (21 mg, 0.025 mmol) in C_6D_6 (0.5 mL). Upon addition a colorless solid precipitated, which was filtered off. 1,1,1-trimethyl-2,2,2-triphenyldisilane was detected as the only product by ^1H NMR spectroscopy.

1,1,1-Trimethyl-2,2,2-triphenyldisilane

^1H NMR (C_6D_6 , 400.1 MHz): δ 0.24 (s, 9H, $\text{Ph}_3\text{SiSiMe}_3$), 7.17-7.19 (m, 9H, *para/meta*-Ph), 7.60-7.62 (m, 6H, *ortho*-Ph).

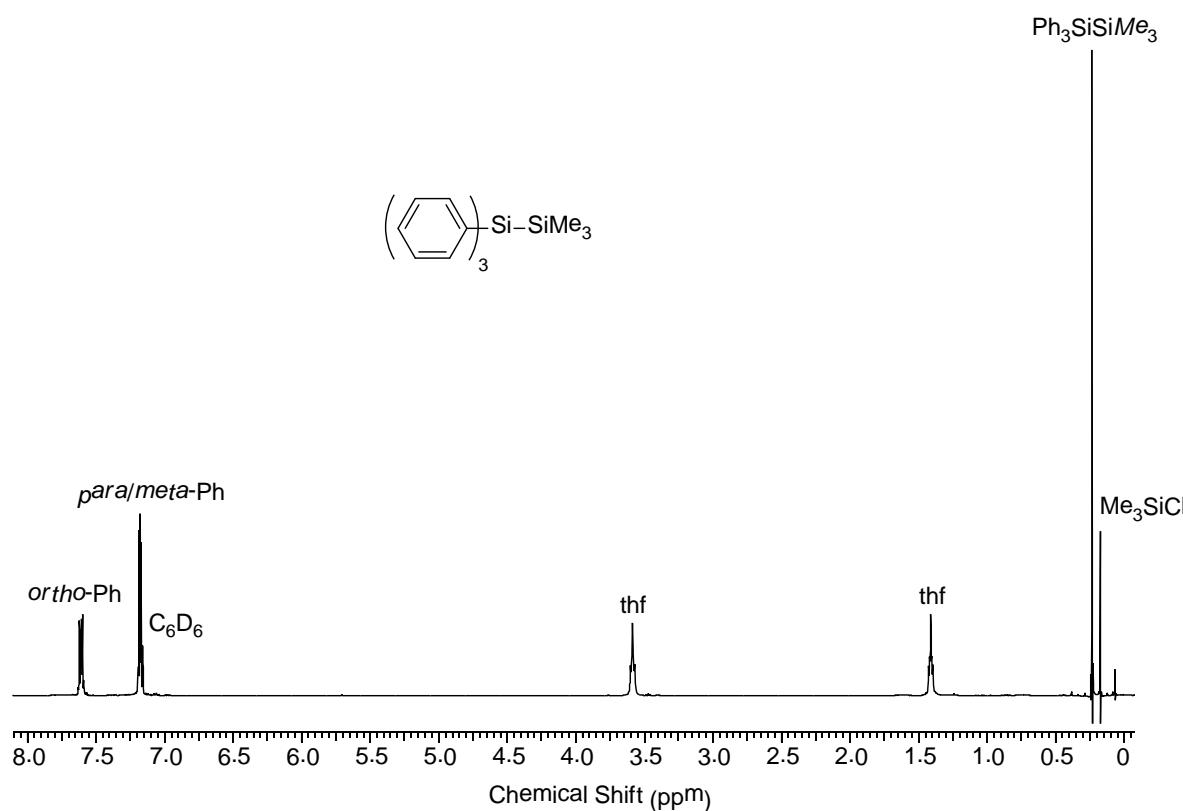


Figure S12 ^1H NMR spectrum of **2a** in C_6D_6 at 25°C after reaction with Me_3SiCl .

Reaction of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (2a**) with H_2 .** A solution of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (**2a**) (21 mg, 0.025 mmol) in C_6D_6 (0.5 mL) was degassed three times with freeze-pump-thaw cycles and refilled with H_2 (1 bar). The conversion to triphenylsilane was complete after 4 h at 60°C . Besides triphenylsilane, an unknown species was detected by ^1H NMR spectroscopy and the broad signal (4 – 5.5 ppm) assigned to a calcium hydride species $[\text{CaH}_2(\text{L})_n]_m$ (**3**).³

Triphenylsilane²

^1H NMR (C_6D_6 , 400.1 MHz): δ 5.71 (s, 1H, Ph_3SiH), 7.12–7.19 (m, 9H, *para/meta-Ph*), 7.58–7.60 (m, 6H, *ortho-Ph*).

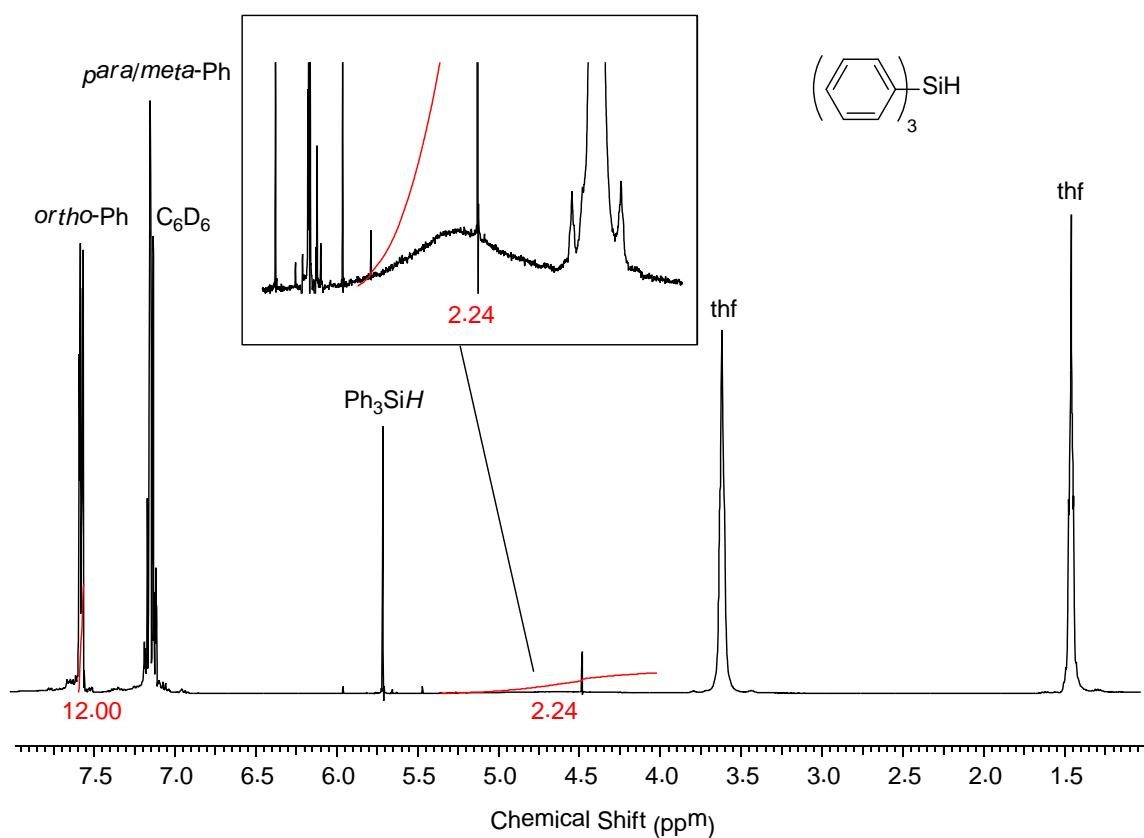


Figure S13 ¹H NMR spectrum of **2a** in C_6D_6 at 25 °C after reaction with H_2 .

Reaction of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (2a**) with 1,1-DPE.** A solution of 1,1-DPE (9 mg, 0.05 mmol) in C_6D_6 (0.25 mL) was added to a solution of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (**2a**) (21 mg, 0.025 mmol) in C_6D_6 (0.25 mL). The reaction mixture turned red and the reaction was followed by ¹H NMR spectroscopy. The conversion to the product bis{1,1-diphenyl-2-(triphenylsilyl)ethyl}calcium **4** was complete after 1 h at 60 °C.

¹H NMR (C_6D_6 , 400.1 MHz): δ 1.27 (m, 16H, *thf*), 2.79 (s, 4H, CH_2), 3.36 (m, 16H, *thf*), 5.74-5.77 (m, 4H, *para*- Ph_{DPE}), 6.49 (m, 8H, *meta*- Ph_{DPE}), 6.65-6.67 (m, 8H, *ortho*- Ph_{DPE}), 7.18-7.21 (m, 18H, *para/meta*-Ph), 7.76-7.78 (m, 12H, *ortho*-Ph). ¹³C{¹H} NMR (C_6D_6 , 100.6 MHz): δ 21.10 (CH_2), 25.86 (*thf*), 69.13 (*thf*), 87.57 (C_{Ca}), 107.67 (*para*- Ph_{DPE}), 119.23 (*ortho*- Ph_{DPE}), 128.21 (*para/meta*-Ph), 129.57 (*para/meta*-Ph), 129.94 (*meta*- Ph_{DPE}), 136.98 (*ortho*-Ph), 137.53 (*ipso*-Ph), 141.74 (*ipso*- Ph_{DPE}).

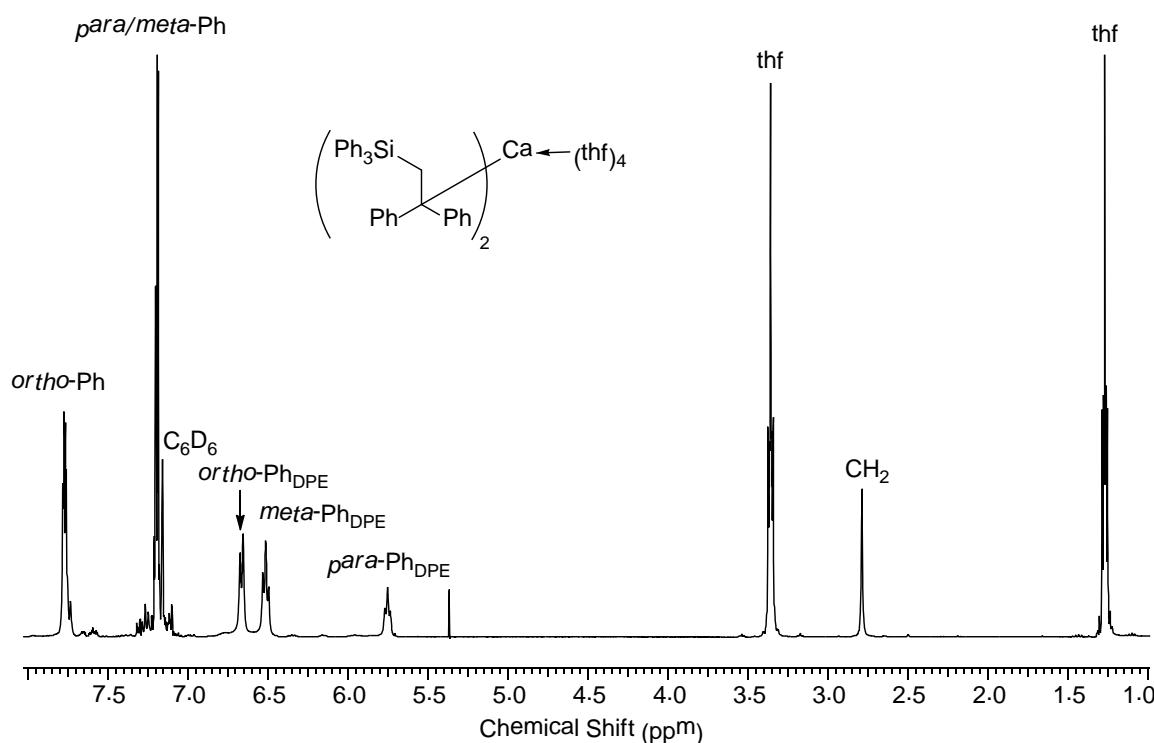


Figure S14 ^1H NMR spectrum of **2a** in C_6D_6 at 25 °C after reaction with DPE.

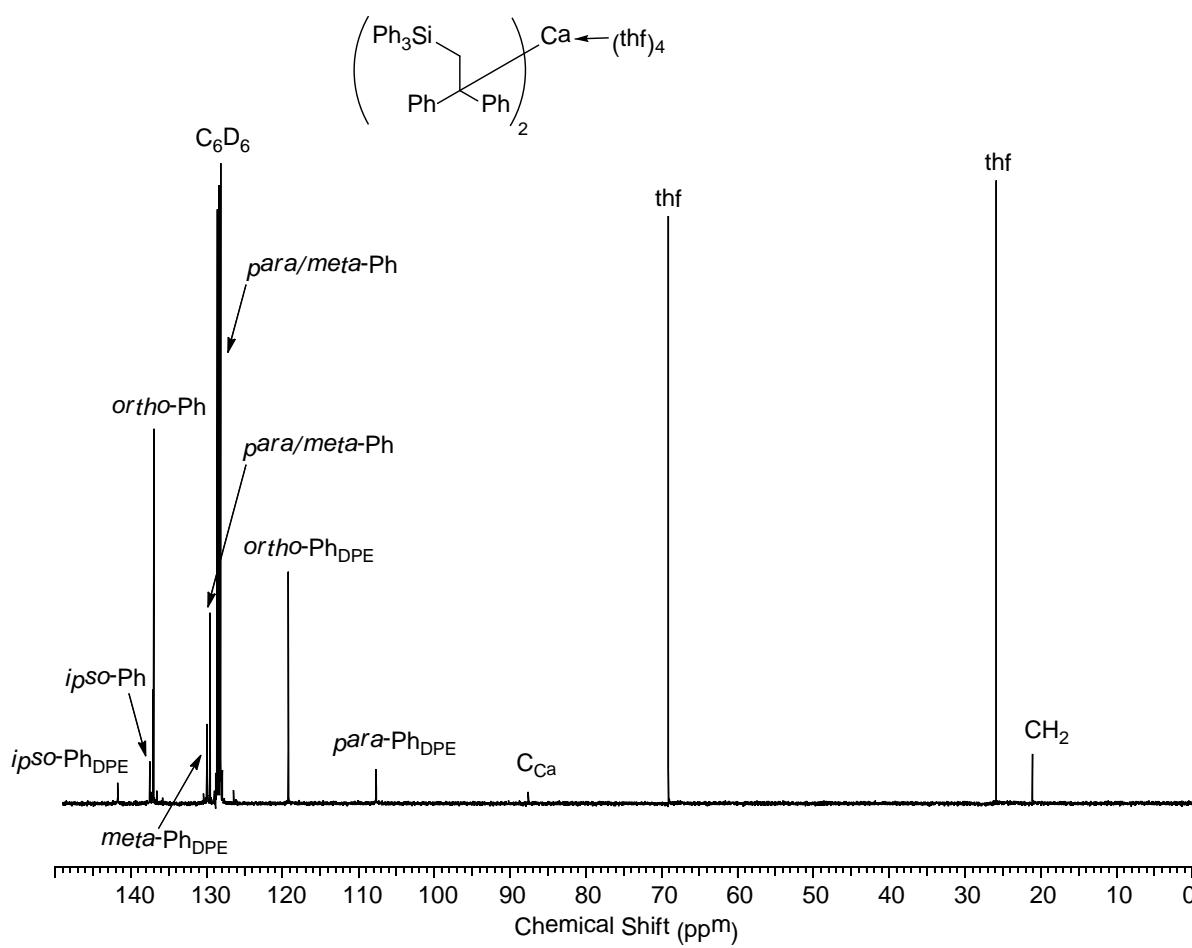


Figure S15 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2a** in C_6D_6 at 25 °C after reaction with DPE.

Reaction of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (2a**) with pyridine.** $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (**2a**) (21 mg, 0.025 mmol) was dissolved in pyridine (0.5 mL) and heated for 5 min. at 60 °C. The reaction mixture turned immediately orange. The excess of pyridine was removed to give an orange powder, which was analyzed by ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectroscopy.

4-Triphenylsilylpyridin

^1H NMR (d_5 -pyridine, 400.1 MHz): δ 7.44-7.48 (m, 6H, *meta*-Ph), 7.51-7.55 (m, 3H, *para*-Ph), 7.54 (d, $^3J_{\text{HH}}$ 5.77 Hz, 2H, *meta*-Ph_{Py}), 7.66-7.69 (m, 6H, *ortho*-Ph), 8.80 (d, $^3J_{\text{HH}}$ 5.77 Hz, 2H, *ortho*-Ph_{Py}). $^{13}\text{C}\{^1\text{H}\}$ NMR (d_5 -pyridine, 100.6 MHz): δ 129.15 (*meta*-Ph), 131.05 (*para*-Ph), 131.51 (*meta*-Ph_{Py}), 133.46 (*ipso*-Ph), 137.14 (*ortho*-Ph), 144.92 (*para*-Ph_{Py}), 150.08 (*ortho*-Ph_{Py}).

Bis(1,4-dihydro-1-pyridyl)calcium (**5**)

^1H NMR (d_5 -pyridine, 400.1 MHz): δ 4.02 (br s, 4H, *para*-Ph_{DHP}), 4.29 (br s, 4H, *meta*-Ph_{DHP}), 6.46 (br s, 4H, *ortho*-Ph_{DHP}). $^{13}\text{C}\{^1\text{H}\}$ NMR (d_5 -pyridine, 100.6 MHz): δ 27.61 (*para*-Ph_{DHP}), 90.90 (*meta*-Ph_{DHP}), 142.94 (*ortho*-Ph_{DHP}).

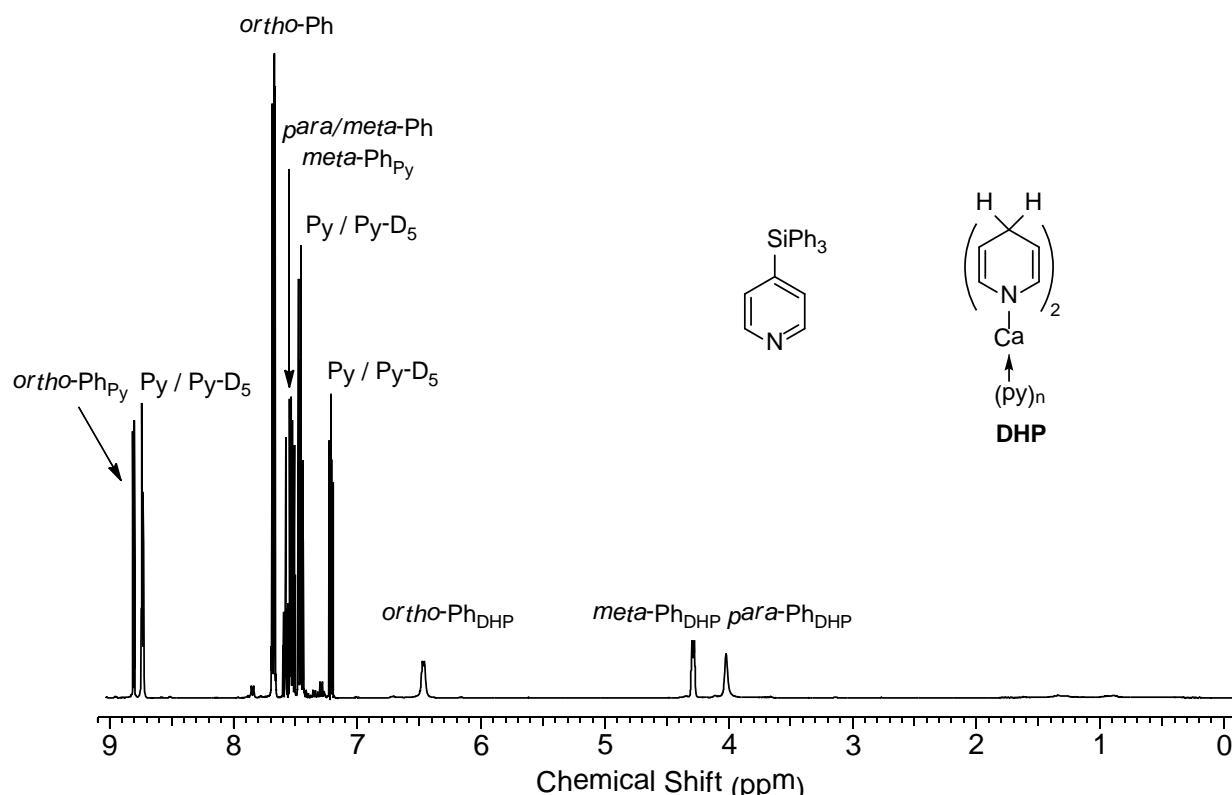


Figure S16 ^1H NMR spectrum of **2a** in d_5 -pyridine at 25 °C after reaction with pyridine.

Hydrosilylation of olefins. Hydrosilylation experiments were performed as follows: A solution of $[\text{Ca}(\text{SiPh}_3)_2(\text{thf})_4]$ (**2a**) (2 mg, 2.5 μmol) in $[\text{D}_8]\text{THF}$ (0.5 mL) was treated with

olefin (0.1 mmol). Immediately the reaction mixture turned deep red. Silane (0.11 mmol) was added and the reaction mixture was heated for the indicated period of time in a Young's NMR tube. The conversion of the substrate was determined by *in situ* ^1H NMR spectroscopy of the reaction mixture.

X-ray Crystallography

X-ray diffraction data was collected at 100 K with a Bruker AXS area detector with Mo K α radiation (λ 0.71073 Å). The SADABS program package was used for the data collection and unit cell determination.⁴ The structures were solved by direct methods using the SHELXS-97 program and refined with the SHELXL-97 software by full matrix least-square procedures based on F^2 .⁵ CCDC 963862 (**2a**) and 963863 (**2b**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

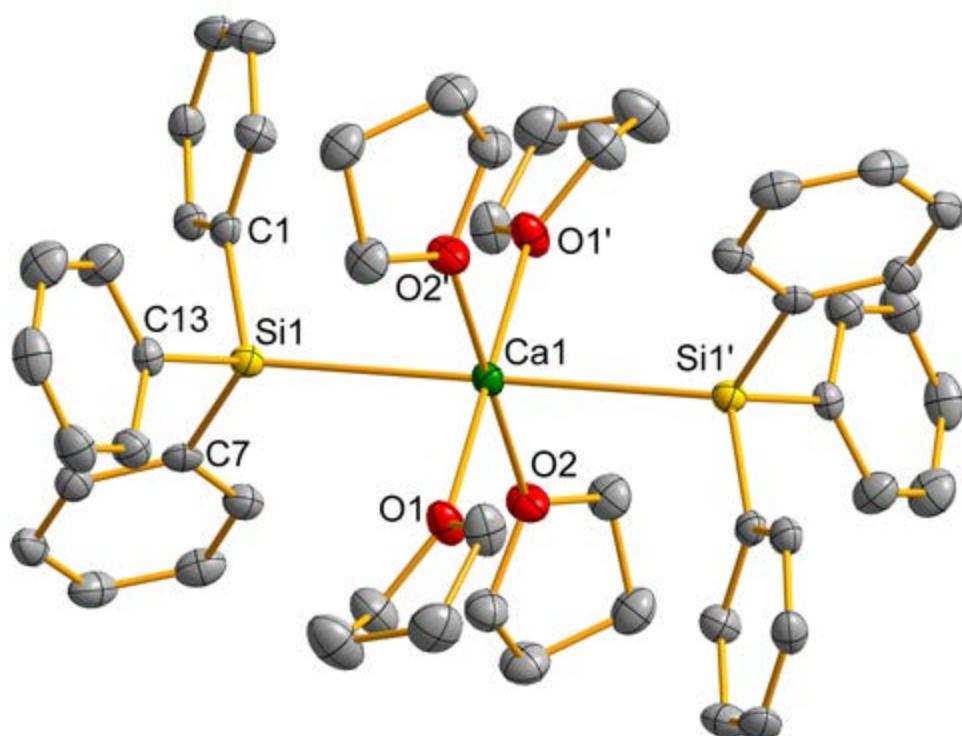


Figure 17 Molecular structure of **2a**. Displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Ca1–Si1 3.1503(8), Ca1–O1 2.438(2), Ca1–O2 2.3838(19), Si1–Ca1–Si1' 180.00, Si1–Ca1–O1 89.64(5), Si1–Ca1–O2 86.56(5), Ca1–Si1–C1 108.73(8), Ca1–Si1–C7 122.11(8), Ca1–Si1–C13 115.38(8).

Crystal data and structure refinement for complex **2a**.

Bond precision: C-C = 0.0042 Å Wavelength=0.71073

Cell: a=10.137(1) b=11.833(2) c=20.015(2)
alpha=90 beta=105.746(6) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2310.7(5)	2310.7(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C18 H15 Si), 4(C4 H8 O), Ca	C52 H62 Ca O4 Si2
Sum formula	C52 H62 Ca O4 Si2	C52 H62 Ca O4 Si2
Mr	847.28	847.28
Dx,g cm-3	1.218	1.218
Z	2	2
Mu (mm-1)	0.232	0.232
F000	908.0	908.0
F000'	909.10	
h,k,lmax	12,14,25	12,14,25
Nref	4754	4740
Tmin,Tmax	0.970,0.975	0.960,0.975
Tmin'	0.959	
Correction method	= MULTI-SCAN	
Data completeness	= 0.997	Theta(max) = 26.430
R(reflections)	= 0.0545(3205)	wR2(reflections) = 0.1183(4740)
S	= 1.033	Npar = 268

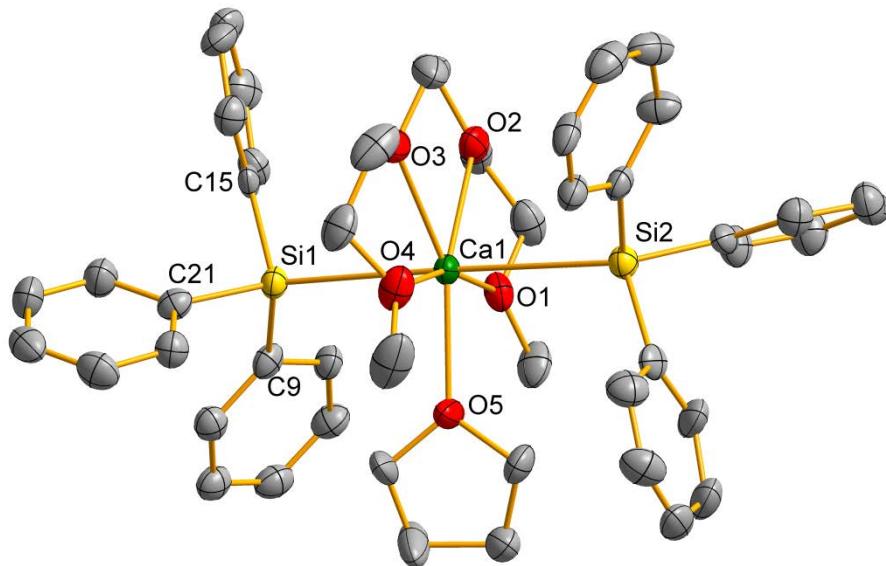


Figure S18 Molecular structure of triglyme adduct **2b**. Displacement ellipsoids are shown at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Ca1–Si1 3.175(3), Ca1–Si2 3.242(3), Ca1–O1 2.492(5), Ca1–O5 2.399(5), Si1–Ca1–Si2 178.24(7), Si1–Ca1–O1 84.85(12), Si1–Ca1–O5 87.17(12).

Crystal data and structure refinement for complex **2b.**

Bond precision: C-C = 0.0117 Å Wavelength=0.71073

Cell: a=9.408(3) b=15.948(5) c=14.884(3)
alpha=90 beta=106.145(5) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2145.1(11)	2145.1(11)
Space group	P c	P 1 c 1
Hall group	P -2yc	-P 2yc
Moiety formula	2(C18 H15 Si), C8 H18 O4, C4 H8 O, C48 H56 Ca O5 Si2 Ca	
Sum formula	C48 H56 Ca O5 Si2	C48 H56 Ca O5 Si2

Mr	809.19	809.19
Dx,g cm-3	1.253	1.253
Z	2	2
Mu (mm-1)	0.248	0.248
F000	864.0	864.0
F000'	865.10	
h,k,lmax	11,20,18	11,19,18
Nref	8924[4472]	8795
Tmin,Tmax	0.931,0.956	0.929,0.957
Tmin'	0.928	

Correction method= MULTI-SCAN

Data completeness= 1.97/0.99 Theta(max)= 26.540

R(reflections)= 0.0765(4633) wR2(reflections)= 0.2242(8795)

S = 0.959 Npar= 508

Computational Details

Calculations were carried out at the DFT level using the hybrid functional B3PW91⁶ with the Gaussian 03⁷ suite of programs. Silicon atoms have been represented by a relativistic effective-core potential (RECP)⁸ from the Stuttgart group and their corresponding optimized basis set. Polarized all-electron triple- ζ 6-311G(d,p)⁹ basis sets were used for Ca, B, C, H, O and N. Geometry optimizations were carried out without any symmetry restriction. The nature of the extrema (minimum) was verified with analytical frequency calculations. The NBO analysis¹⁰ was carried out with an even number of f electrons for the calculations because of the technical requirement.

Cartesian coordinates of the optimized structure

HF= -3004.355744 a.u.
Ca 10.136974 0.000021 -0.000172 0.901044
Si 8.969102 -1.898770 -2.316690 -0.151455
O 7.884186 0.073493 0.982539 -0.578259
O 10.763092 -2.014239 1.237892 -0.573673
C 7.651047 -3.126938 -1.569860 -0.009317
C 6.537345 -3.601988 -2.283947 -0.149178
H 6.376647 -3.262589 -3.304471 0.120699
C 5.630087 -4.497482 -1.717288 -0.115895

H	4.778466	-4.844973	-2.298112	0.112735
C	5.812966	-4.953103	-0.411505	-0.133750
H	5.108396	-5.653920	0.029423	0.111486
C	6.906395	-4.497318	0.323468	-0.123697
H	7.057822	-4.843117	1.344288	0.101692
C	7.801019	-3.590985	-0.250591	-0.162843
H	8.637747	-3.222480	0.341339	0.099500
C	7.965929	-1.088952	-3.774442	-0.004794
C	7.280049	0.118149	-3.548116	-0.165447
H	7.367756	0.600012	-2.575078	0.096686
C	6.491140	0.721820	-4.528480	-0.118630
H	5.963594	1.648451	-4.310454	0.103265
C	6.378450	0.136348	-5.788693	-0.132910
H	5.770721	0.603251	-6.559711	0.111758
C	7.052846	-1.056201	-6.047539	-0.115945
H	6.970055	-1.525200	-7.025585	0.112859
C	7.827646	-1.657008	-5.053857	-0.169042
H	8.335699	-2.591732	-5.278616	0.126352
C	10.138734	-3.143290	-3.243259	0.012911
C	10.326187	-4.466368	-2.801696	-0.174693
H	9.724270	-4.841197	-1.976219	0.113583
C	11.241883	-5.326153	-3.409733	-0.114271
H	11.351692	-6.344734	-3.043328	0.108666
C	12.001624	-4.891798	-4.495270	-0.136580
H	12.709485	-5.561871	-4.976433	0.109575
C	11.830467	-3.589509	-4.964579	-0.112694
H	12.403655	-3.239750	-5.820753	0.107842
C	10.919445	-2.734930	-4.342996	-0.189643
H	10.796845	-1.727528	-4.739062	0.112008
C	6.642225	-0.158582	0.280715	0.023731
H	6.819137	-0.930164	-0.469498	0.176099
H	6.333379	0.770804	-0.218187	0.120601
C	5.650461	-0.553050	1.360384	-0.288672
H	5.779484	-1.610115	1.615876	0.159441
H	4.613748	-0.399181	1.049544	0.145531
C	6.081870	0.353653	2.514641	-0.305268
H	5.674753	1.361775	2.380724	0.148999
H	5.764415	-0.007738	3.496358	0.145546
C	7.603272	0.369519	2.375271	0.028885
H	8.055948	1.329249	2.631124	0.175053
H	8.071142	-0.411129	2.985667	0.126888
C	10.373344	-2.332793	2.593714	0.017603
H	9.300147	-2.562009	2.595922	0.134413
H	10.563629	-1.454196	3.216319	0.172324
C	11.204700	-3.547763	2.985315	-0.295817
H	10.700804	-4.169622	3.729969	0.147090
H	12.164832	-3.227653	3.403156	0.154306
C	11.402876	-4.251138	1.639879	-0.297955
H	12.262189	-4.926836	1.626053	0.148360
H	10.511502	-4.827599	1.369713	0.156268
C	11.579931	-3.075439	0.689637	0.018609

H	12.622036	-2.733644	0.663964	0.133094
H	11.243951	-3.272772	-0.331927	0.175729
Si	11.305042	1.898530	2.316628	-0.151534
O	12.389762	-0.073356	-0.982782	-0.578262
O	9.510147	2.014294	-1.237833	-0.573722
C	12.623043	3.126698	1.569709	-0.009320
C	13.736990	3.601483	2.283589	-0.149232
H	13.897894	3.261909	3.304023	0.120720
C	14.644227	4.496946	1.716843	-0.115893
H	15.496036	4.844236	2.297513	0.112722
C	14.461090	4.952791	0.411176	-0.133746
H	15.165644	5.653579	-0.029821	0.111455
C	13.367425	4.497252	-0.323603	-0.123783
H	13.215799	4.843216	-1.344338	0.101681
C	12.472827	3.590949	0.250538	-0.162885
H	11.635926	3.222615	-0.341255	0.099498
C	12.308391	1.088628	3.774211	-0.004772
C	12.994393	-0.118367	3.547691	-0.165432
H	12.906689	-0.600115	2.574596	0.096665
C	13.783438	-0.722068	4.527925	-0.118688
H	14.311082	-1.648608	4.309744	0.103268
C	13.896141	-0.136745	5.788207	-0.132923
H	14.503974	-0.603676	6.559126	0.111781
C	13.221632	1.055697	6.047243	-0.115974
H	13.304439	1.524591	7.025338	0.112835
C	12.446705	1.656546	5.053683	-0.169017
H	11.938575	2.591192	5.278586	0.126372
C	10.135542	3.143003	3.243437	0.012882
C	9.948128	4.466171	2.802137	-0.174674
H	10.549999	4.841121	1.976683	0.113550
C	9.032530	5.325894	3.410413	-0.114265
H	8.922755	6.344553	3.044212	0.108668
C	8.272845	4.891376	4.495921	-0.136614
H	7.565063	5.561401	4.977267	0.109587
C	8.443956	3.588983	4.964964	-0.112736
H	7.870801	3.239090	5.821105	0.107828
C	9.354882	2.734475	4.343150	-0.189687
H	9.477449	1.726987	4.739012	0.111995
C	13.631756	0.158657	-0.280985	0.023741
H	13.454828	0.930016	0.469452	0.176076
H	13.940722	-0.770840	0.217633	0.120605
C	14.623406	0.553530	-1.360614	-0.288693
H	14.494293	1.610668	-1.615760	0.159459
H	15.660154	0.399631	-1.049906	0.145529
C	14.191961	-0.352826	-2.515127	-0.305194
H	14.599094	-1.360987	-2.381544	0.149019
H	14.509352	0.008874	-3.496751	0.145528
C	12.670575	-0.368756	-2.375671	0.028908
H	12.217876	-1.328371	-2.631903	0.175089
H	12.202673	0.412177	-2.985684	0.126902
C	9.899930	2.333350	-2.593529	0.017588

H	10.973120	2.562613	-2.595638	0.134409
H	9.709701	1.454970	-3.216456	0.172330
C	9.068535	3.548433	-2.984696	-0.295766
H	9.572363	4.170527	-3.729200	0.147094
H	8.108369	3.228446	-3.402557	0.154305
C	8.870456	4.251379	-1.639027	-0.297987
H	8.011151	4.927082	-1.624930	0.148327
H	9.761852	4.827751	-1.368744	0.156291
C	8.693448	3.075384	-0.689140	0.018716
H	7.651332	2.733634	-0.663449	0.133115
H	9.029556	3.272381	0.332446	0.175739

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