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1 General Considerations

Et_2O (Sigma-Aldrich), THF (Roth, 99%), n-hexane (Roth, 98%) and toluene (Roth, 99%) were dried over sodium and distilled prior to use. C_6D_6 and THF-D8 (Eurisotop) were dried over sodium and distilled prior to use.

Starting materials were prepared according to literature protocols: RH,[1] $[Ca\{N(SiMe_3)_2\}_2(THF)_2]$,[2] $Yb\{N(SiMe_3)_2\}_2(THF)$[3], $PhSiD_3$.[4]

NMR spectra were acquired on a Bruker Avance 400 MHz spectrometer. Reported chemical shifts are referenced to the ^1H and ^{13}C NMR resonances of the deuterated solvent.[5] Coupling constants *J* are given in Hertz as positive values regardless of their real individual sign. ^1H, ^{11}B, ^{13}C, ^{15}N, ^{19}F, ^{29}Si NMR spectra were obtained at 400.1, 128.4, 100.6, 40.6, 376.5, 79.5 MHz, respectively.

IR spectra were recorded on a Bruker Alpha spectrometer using the attenuated total reflection (ATR) technique on powdered samples.

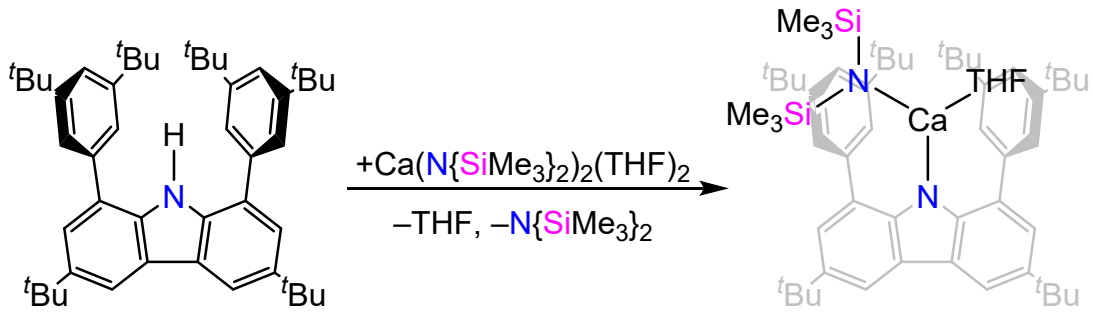
Raman spectra were recorded in the region 4000-20 cm^{-1} on a *Bruker MultiRam* spectrometer equipped with a Nd:YAG laser (λ = 1064 nm) and a germanium detector at a resolution of 2 cm^{-1}. The powdered crystalline sample materials were flame sealed in a glass tube. The laser energy was adjusted to 100 mW.

Elemental analyses were obtained with a Vario Micro Cube (Elementar Analysensysteme GmbH) in the institutional technical laboratories of the Karlsruhe Institute of Technology (KIT).

Single crystals were mounted in perfluoropolyalkyl ether oil on a cryo loop and then brought into the cold nitrogen stream of a low-temperature device (Oxford Cryosystems Cryostream unit) so that the oil solidified. Diffraction data were collected using a Stoe IPDS II diffractometer and graphite-monochromated Mo-Kα (0.71073 Å) radiation or a Stoe STADIVARI diffractometer and Ga-Kα (1.34134 Å) radiation. The structures were solved by direct methods with SHELXS[6] or intrinsic phasing with SHELXT[7] followed by full-matrix least-squares refinement using SHELXL-2018/3[8] and the ShelXle GUI.[9] All non-hydrogen atoms were refined anisotropically. The contribution of the hydrogen atoms, in their calculated positions, was included in the refinement using a riding model.

2 Syntheses

2.1 [(^{dtbp}Cbz)CaN(SiMe$_3$)$_2$(THF)] (**1Ca**)



As solids, ^{dtbp}CbzH (400 mg, 0.610 mmol) and Ca[N(SiMe$_3$)$_2$]$_2$(THF)$_2$ (296 mg, 0.586 mmol) were combined. To the mixture, 9 mL of toluene were added via syringe. The resulting solution quickly turned dark yellow and was stirred overnight at ambient temperature. Then, the solvent was evaporated and the crude product was treated with 13 mL *n*-hexane, filtered and concentrated until approximately 3 mL. Within one night, suitable crystals were obtained. The crystals were washed with 1 mL *n*-hexane and briefly dried in vacuo (176 mg, 0.189 mmol). A second fraction could be obtained by concentrating the mother liquor (46 mg, 0.049 mmol). Crystalline yield: 222 mg, 0.239 mmol, 41%. The characterisation data were obtained from the crystalline material.

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = -0.18 (s, 18 H, Si(C*H*$_3$)$_3$), 0.99 (br, 4 H, OCC*H*$_2$), 1.43 (s, 36 H, Ar-C(C*H*$_3$)$_3$), 1.52 (s, 18 H, Carb-C(C*H*$_3$)$_3$), 2.83 (br, 4 H, OC*H*$_2$), 7.62 (t, 2 H, $^4J_{HH}$ = 1.9 Hz, *p*-C*H*), 7.64 (d, 2 H, $^4J_{HH}$ = 2.0 Hz, C^{2,7}*H*), 8.10 (d, 4 H, $^4J_{HH}$ = 1.9 Hz, *o*-C*H*), 8.52 (d, 2 H, $^4J_{HH}$ = 2.0 Hz, C^{2,7}*H*).

^{13}C{^{1}H} NMR (100.7 MHz, C_6D_6): δ (ppm) = 5.26 (s, Si(*C*H$_3$)$_3$), 24.72 (s, OC*C*H$_2$), 31.97 (s, Ar-C(*C*H$_3$)$_3$), 32.46 (s, Carb-C(*C*H$_3$)$_3$), 34.76 (s, Carb-*C*(CH$_3$)$_3$), 35.32 (s, Ar-*C*(CH$_3$)$_3$), 69.04 (s, O*C*H$_2$), 116.18 (s, *C*H), 123.29 (s, *C*H), 123.84 (s, *C*H), 125.42 (s, *C*H), 127.03 (s), 139.46 (s), 142.60 (s), 147.34 (s), 152.71 (s).

^{29}Si NMR (79.5 MHz, C_6D_6): δ (ppm) = -15.6 (s, *Si*(CH$_3$)$_3$).

EA found (calc. for $C_{58}H_{90}N_2OSi_2Ca$): C 74.66 (75.10), H 9.69 (9.78), N 2.69 (3.02).

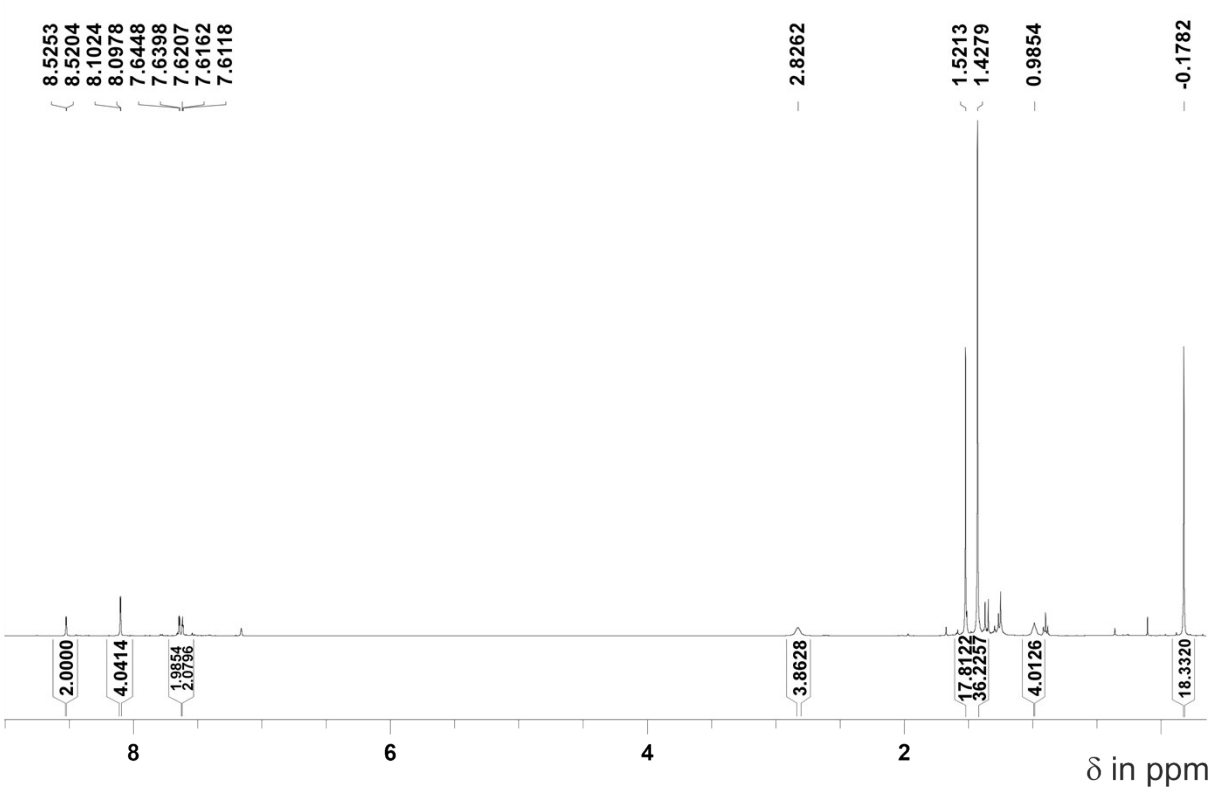


Figure S1: ^{1}H NMR spectrum of **1Ca**.

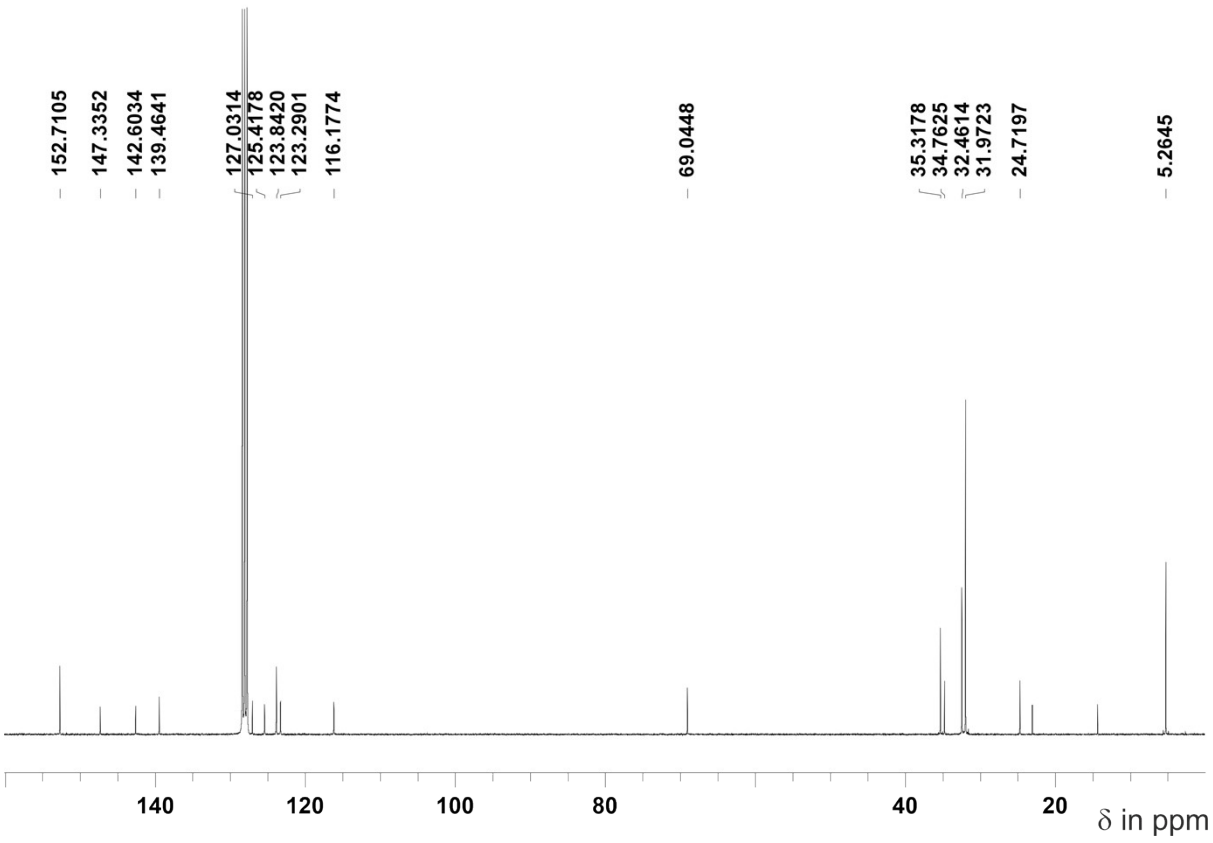


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **1Ca**.

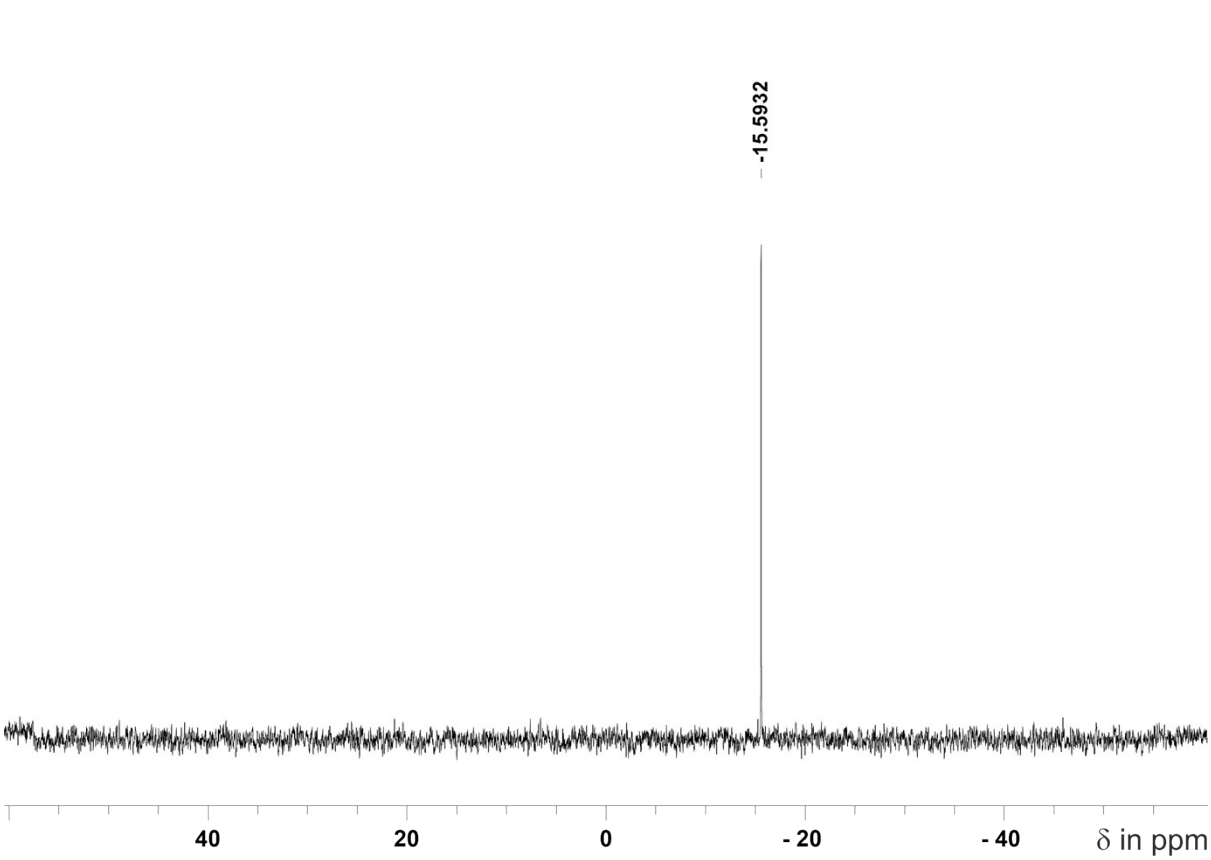


Figure S3: $^{29}Si\{^{1}H\}$ NMR spectrum of **1Ca**.

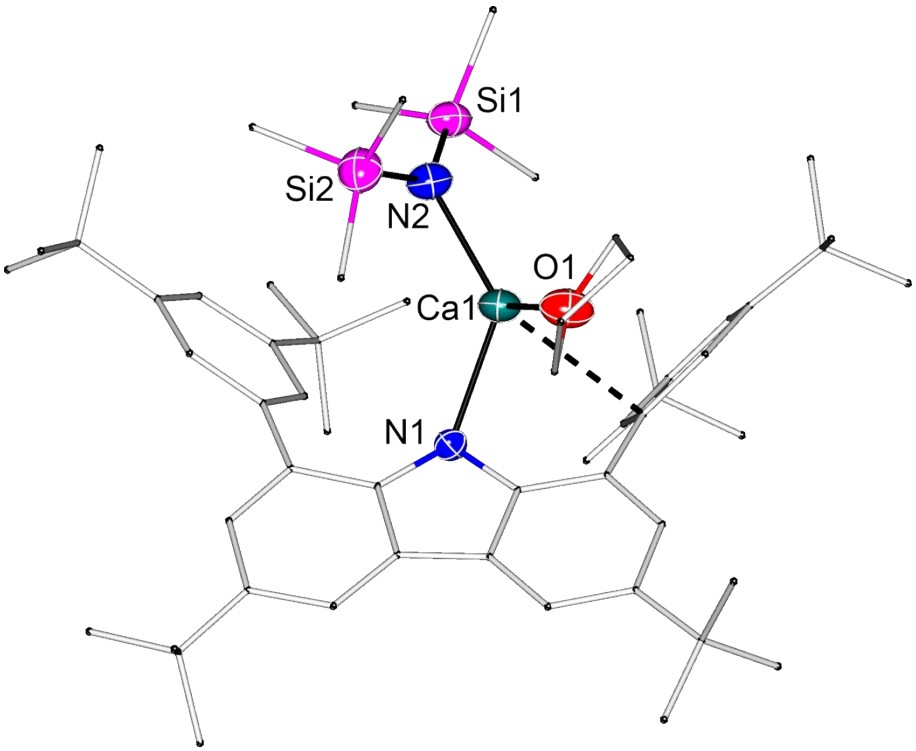
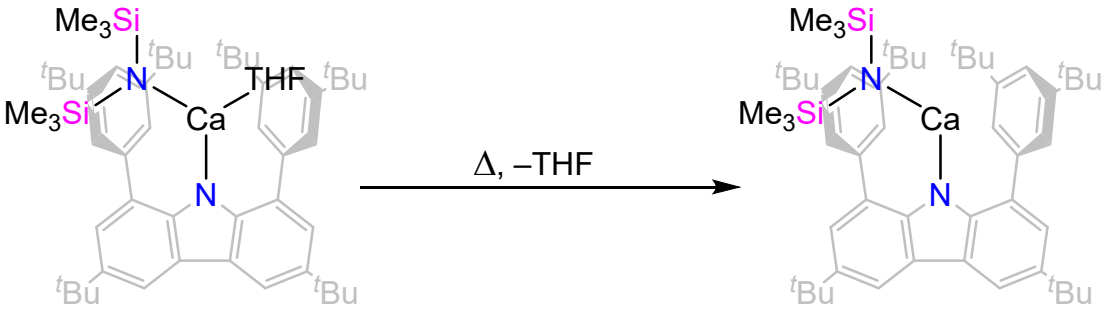


Figure S4: Molecular structure of **1Ca**.

2.2 [(^{dtbp}Cbz)CaN(SiMe$_3$)$_2$] (2Ca)



a) A finely ground sample of (^{dtbp}Cbz)CaN(SiMe$_3$)$_2$(THF) (120 mg, 0.129 mmol) was dried for 20 hours at 120 °C in a dynamic rotary vane pump vacuum. No colour change occurred. The crude product (107 mg, 0.125 mmol) was recrystallised from a minimal amount of *n*-hexane to obtain single crystals suitable for XRD experiments.

b) Alternatively, transamination with ^{dtbp}CbzH and Ca[N(SiMe$_3$)$_2$]$_2$ works as well. Ca[N(SiMe$_3$)$_2$]$_2$ is prepared by drying Ca[N(SiMe$_3$)$_2$]$_2$(THF)$_2$ at 115 °C for nine hours. ^{dtbp}CbzH (562 mg, 0.857 mmol) and Ca[N(SiMe$_3$)$_2$]$_2$ (308 mg, 0.853 mmol) were dissolved in 11 mL toluene and the mixture was stirred overnight at ambient temperature. All volatiles were removed in *vacuo* and the residue was treated with 22 mL *n*-hexane, filtered and concentrated to a few milliliters. Crystallization occured within one night. The yellow crystals were washed with *n*-hexane and briefly dried. Crystalline yield: 384 mg, 0.449 mmol, 52%. The characterisation data were obtained from the crystalline material.

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = -0.26 (s, 18 H, Si(C*H*$_3$)$_3$), 1.32 (s, 36 H, Ar-C(C*H*$_3$)$_3$), 1.56 (s, 18 H, Carb-C(C*H*$_3$)$_3$), 7.59 (t, 2 H, $^4J_{HH}$ = 1.9 Hz, *p*-C*H*), 7.67 (d, 2 H, $^4J_{HH}$ = 2.0 Hz, C^{2,7}*H*), 7.99 (d, 4 H, $^4J_{HH}$ = 1.9 Hz, *o*-C*H*), 8.61 (d, 2 H, $^4J_{HH}$ = 2.0 Hz, C^{2,7}*H*).

^{13}C{^{1}H} NMR (100.7 MHz, C_6D_6): δ (ppm) = 5.24 (s, Si(*C*H$_3$)$_3$), 31.91 (s, Ar-C(*C*H$_3$)$_3$), 32.51 (s, Carb-C(*C*H$_3$)$_3$), 34.82 (s, Carb-*C*(CH$_3$)$_3$), 35.37 (s, Ar-*C*(CH$_3$)$_3$), 116.47 (s, *C*H), 123.31 (s, *C*H), 123.71 (s, *C*H), 124.60 (s, *C*H), 126.69 (s), 127.57 (s), 139.43 (s), 143.61 (s), 147.54 (s), 153.39 (s).

^{29}Si NMR (79.5 MHz, C_6D_6): δ (ppm) = -15.5 (s, *Si*(CH$_3$)$_3$).

IR (ATR) ũ (cm^{-1}) = 2954 (S), 2867 (VW), 2229 (VW), 2199 (VW), 2180 (VW), 2123 (VW), 2083 (VW), 1990 (VW), 1978 (VW), 1966 (VW), 1589 (W), 1462 (W), 1391 (VW), 1362 (M), 1286 (W), 1237 (S), 1181 (VW), 1151 (VW), 1055 (M), 931 (VW), 867 (S), 821 (VS), 763 (W), 718 (M), 698 (VW), 664 (W), 643 (VW), 595 (W), 566 (VW), 544 (VW), 504 (VW), 467 (W), 426 (W), 411 (W), 390 (M).

EA found (calc. for $C_{54}H_{82}N_2Si_2Ca$): C 75.94 (75.81), H 9.38 (9.66), N 3.12 (3.27).

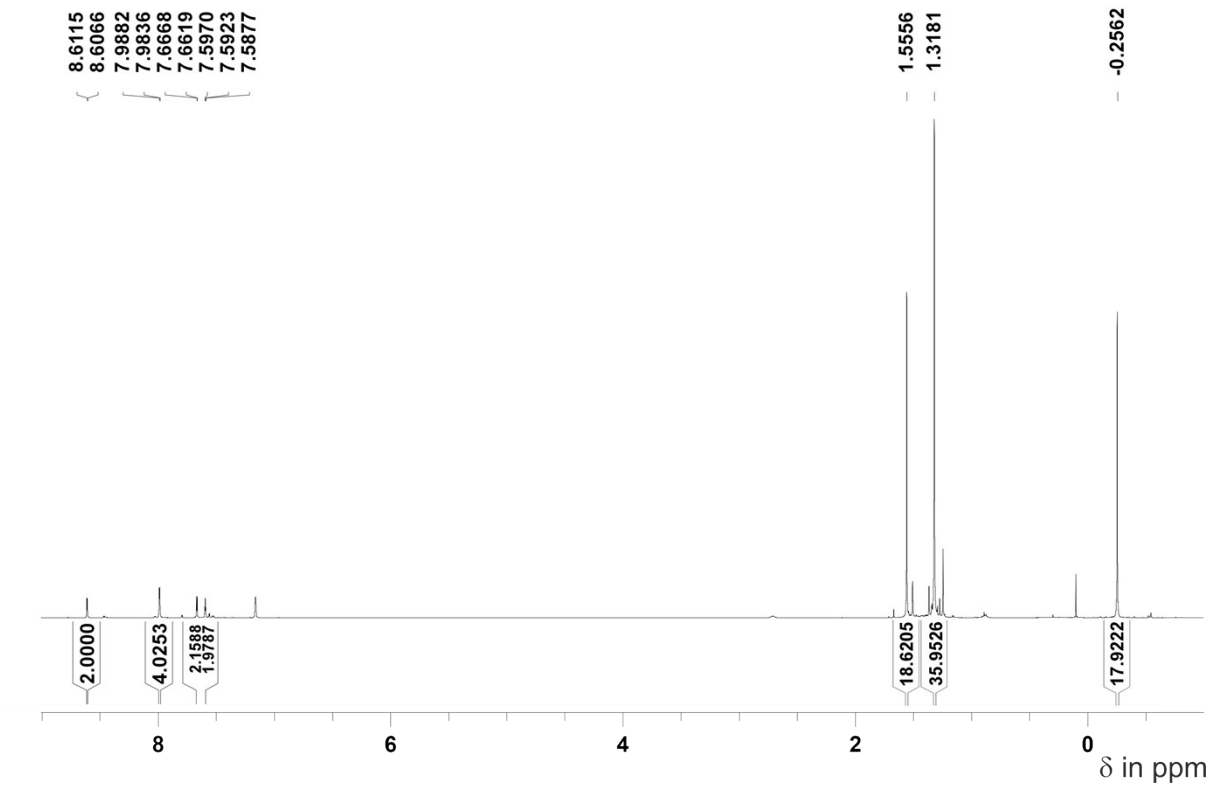


Figure S5: ^{1}H NMR spectrum of **2Ca**.

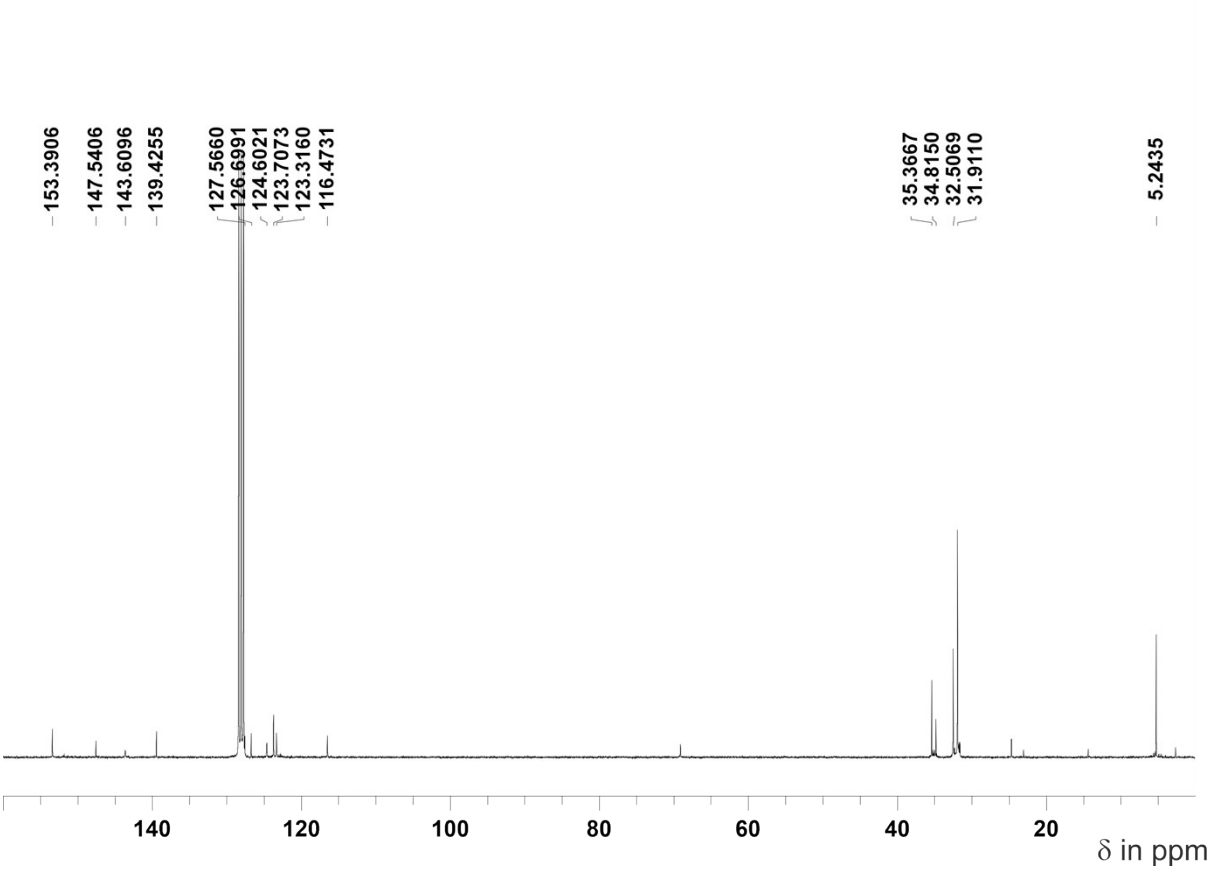


Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of **2Ca**.

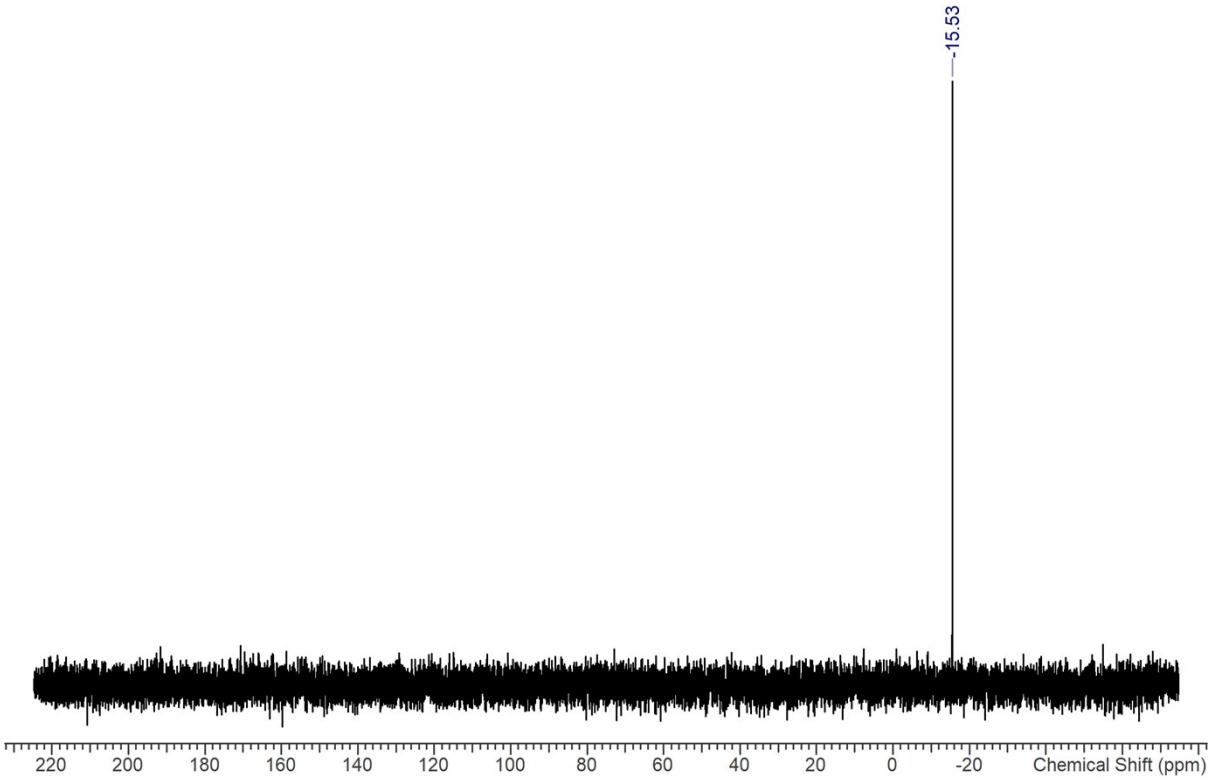


Figure S7: $^{29}Si\{^{1}H\}$ NMR spectrum of **2Ca**.

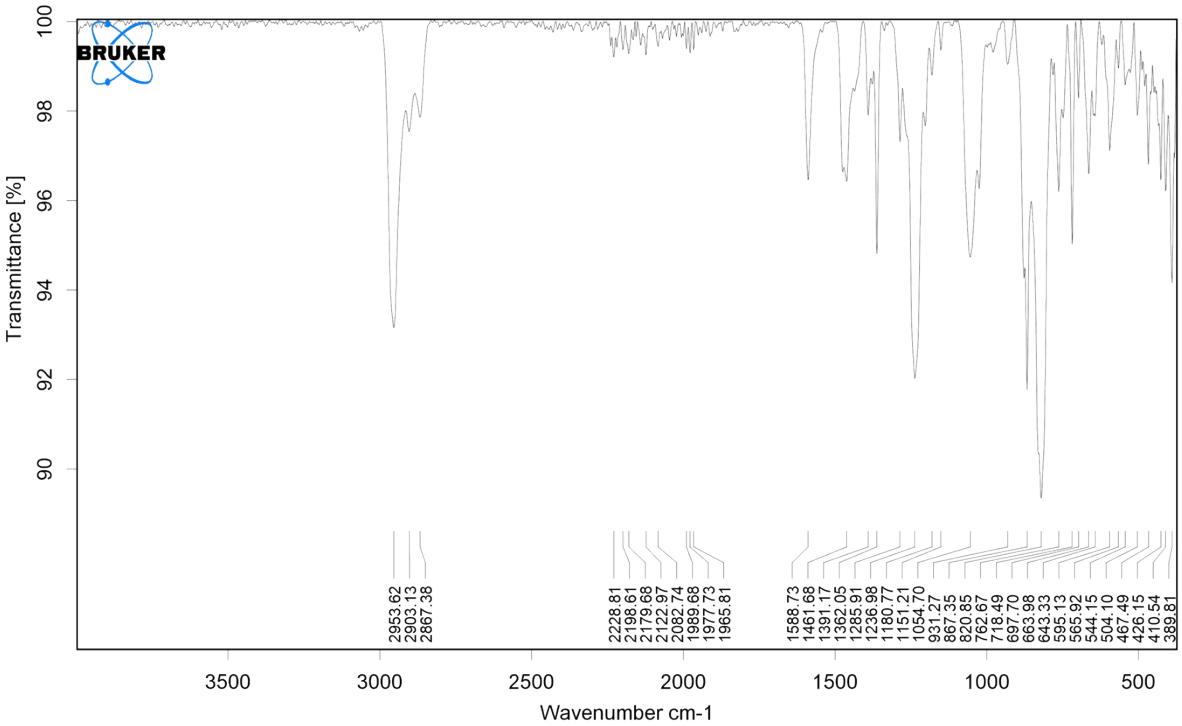


Figure S8: IR spectrum of **2Ca**.

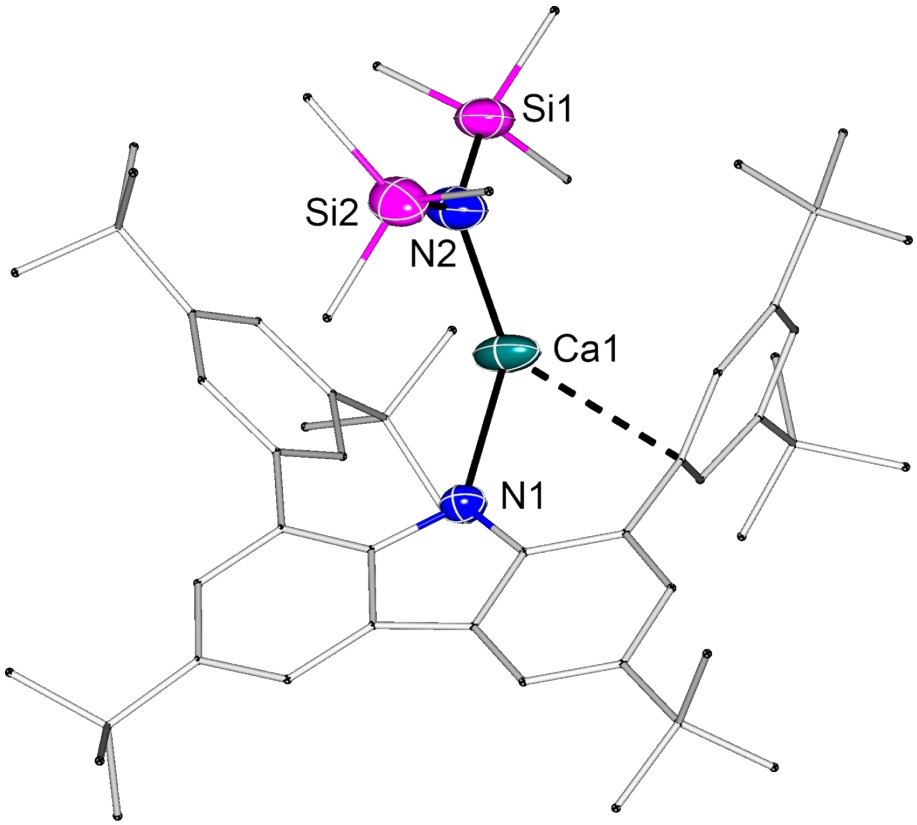
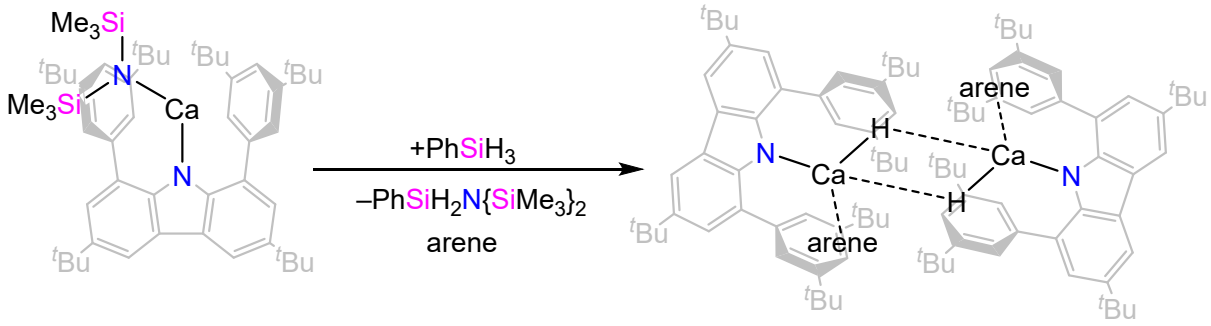


Figure S9: Molecular structure of **2Ca**.

2.3 [(dtbpCbz)Ca(C$_6$H$_6$)H] (**3Ca**·C$_6$H$_6$)



The amide **2Ca** (388 mg, 0.454 mmol) was dissolved in 1.6 mL of benzene. To that solution, phenylsilane (87.7 mg, 100 µL, 0.810 mmol, 1.78 eq.) was added via microsyringe. The mixture was shaken and then left undisturbed overnight. The hydride **3Ca·C$_6$H$_6$** crystallized within one night. Afterwards, the supernatant was removed via syringe, the crystals were washed multiple times with *n*-hexane and briefly dried. Crystalline yield: 153 mg, 0.110 mmol, 48%. The characterisation data were obtained from the crystalline material.

In the same reaction, **1Ca** can be used as starting material, and [dtbpCbzCaH·THF] (**3Ca**·THF) is obtained.

Due to the poor solubility of compound **3Ca**, only ^{1}H NMR solution characterisation was performed.

^{1}H NMR (400 MHz, C$_6$D$_6$): δ (ppm) = 1.46 (br s, 36 H, $\nu_{1/2}$ = 37 Hz, Ar-C(C*H*$_3$)$_3$), 1.53 (s, 18 H, $\nu_{1/2}$ = 1.3 Hz, Carb-C(C*H*$_3$)$_3$), **2.07** (s, 1 H, $\nu_{1/2}$ = 7.1 Hz, Ca*H*), 7.46 (d, 2 H, $^4J_{HH}$ = 1.9 Hz, C^{2,7}*H*), 7.58 (br s, 2 H, $\nu_{1/2}$ = 4.6 Hz, *p*-C*H*), 7.87 (br s, 4 H, $\nu_{1/2}$ = 5.9 Hz, *o*-C*H*), 8.51 (d, 2 H, $^4J_{HH}$ = 1.9 Hz, C^{4,5}*H*).

MP (°C): 210 (darkened), 280 (dec.).

IR (ATR) ũ (cm^{-1}) = 386 (M), 404 (W), 417 (W), 459 (W), 500 (M), 519 (W), 556 (VS), 644 (M), 679 (S), 699 (S), 707 (S), 714 (S), 785 (M), 825 (W), 846 (M), 866 (S), 899 (W), 933 (W), 981 (W), 1035 (M), 1069 (S), 1151 (W), 1182 (W), 1201 (M), 1230 (S), 1245 (M), 1267 (M), 1286 (M), 1361 (S), 1381 (W), 1392 (M), 1432 (W), 1463 (M), 1476 (M), 1588 (M), 2866 (M), 2903 (M), 2954 (S), 3035 (VW), 3068 (VW).

Raman (cm^{-1}): 69 (100), 93 (93), 150 (45), 210 (25), 222 (25), 251 (13), 368 (8), 391 (7), 433 (7), 519 (8), 550 (19), 609 (7), 619 (6), 700 (7), 783 (15), 798 (6), 825 (26), 854 (11), 868 (7), 883 (7), 897 (11), 924 (26), 999 (50), 1026 (7), 1099 (13), 1151 (11), 1178 (10), 1201 (24), 1253 (37), 1267 (23), 1288 (17), 1317 (80), 1338 (37), 1363 (13), 1396 (16), 1446 (27), 1466 (26), 1550 (19), 1568 (29), 1593 (75), 1616 (14), 2710 (8), 2779 (67), 2866 (22), 2904 (46), 2927 (34), 2960 (43), 3066 (13).

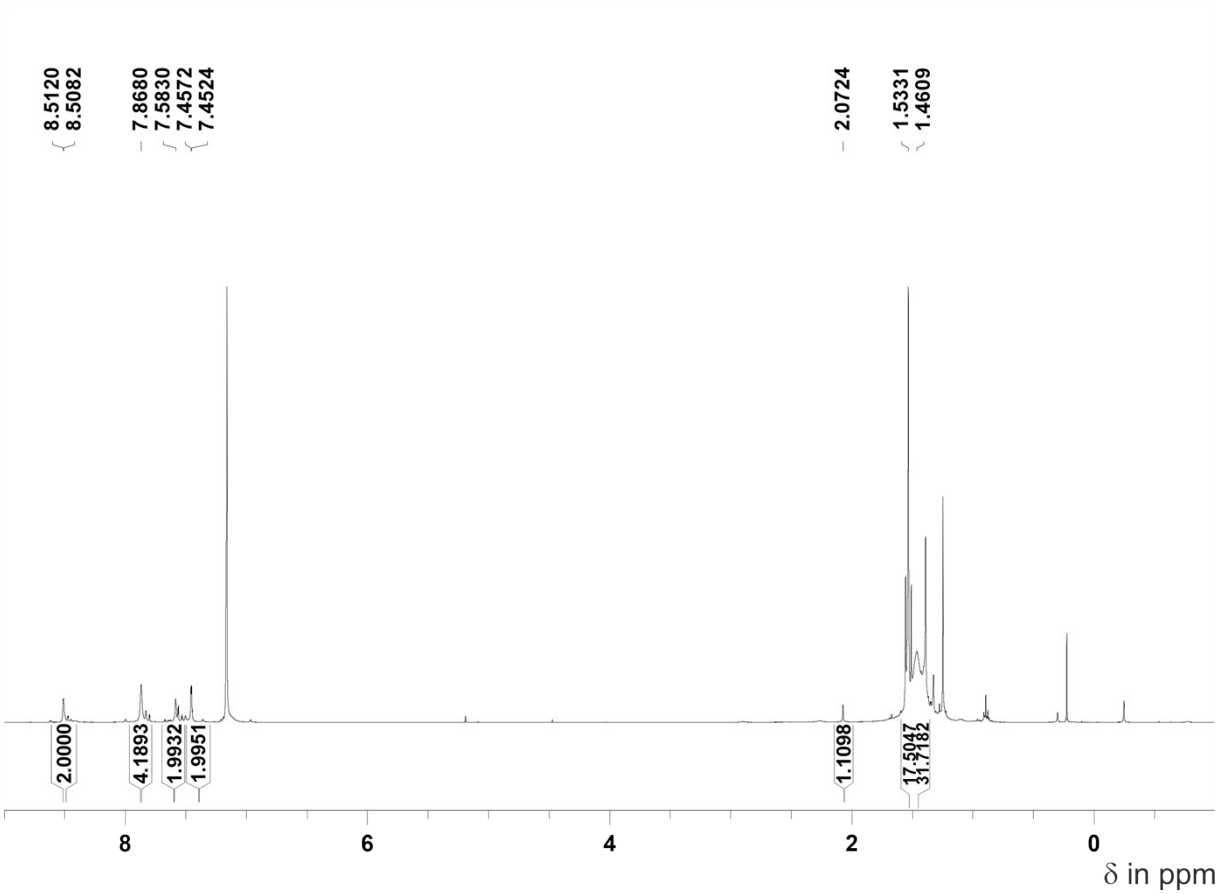


Figure S10: ^{1}H NMR spectrum of **3Ca·C_6H_6**.

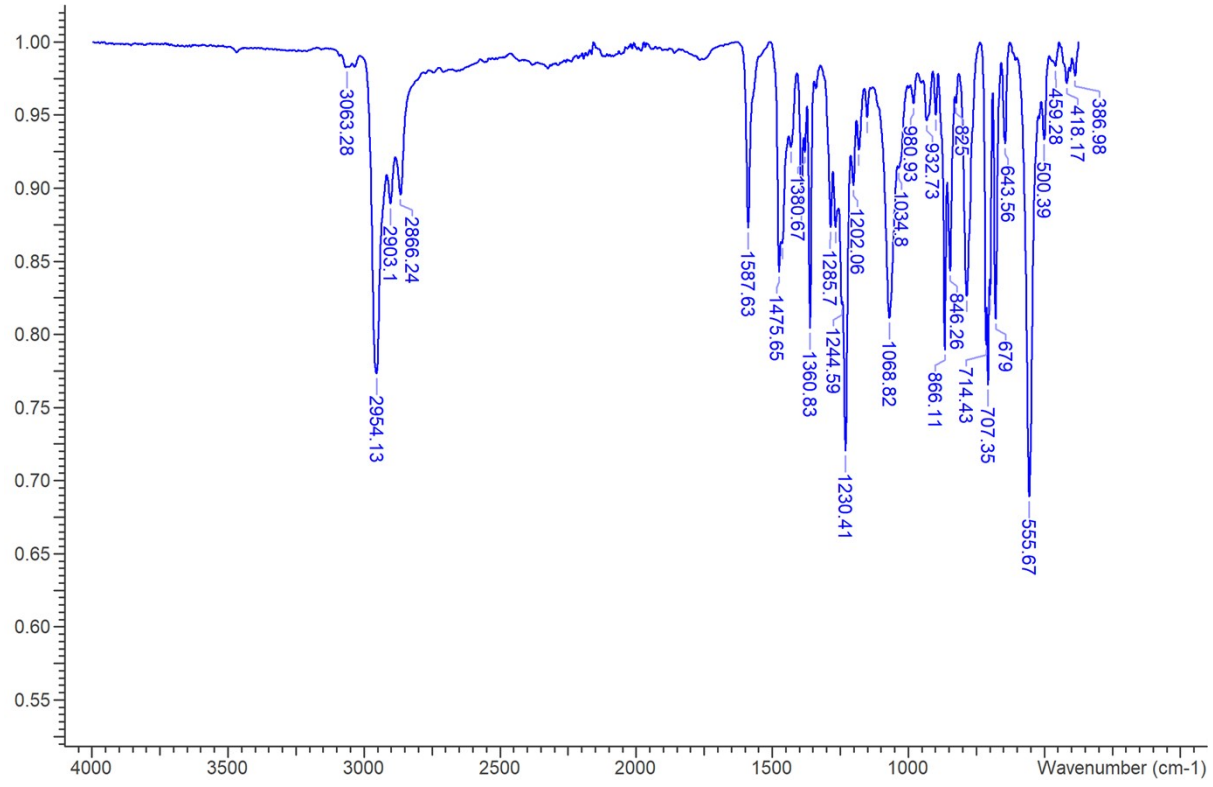


Figure S11: IR spectrum of **3Ca·C_6H_6**.

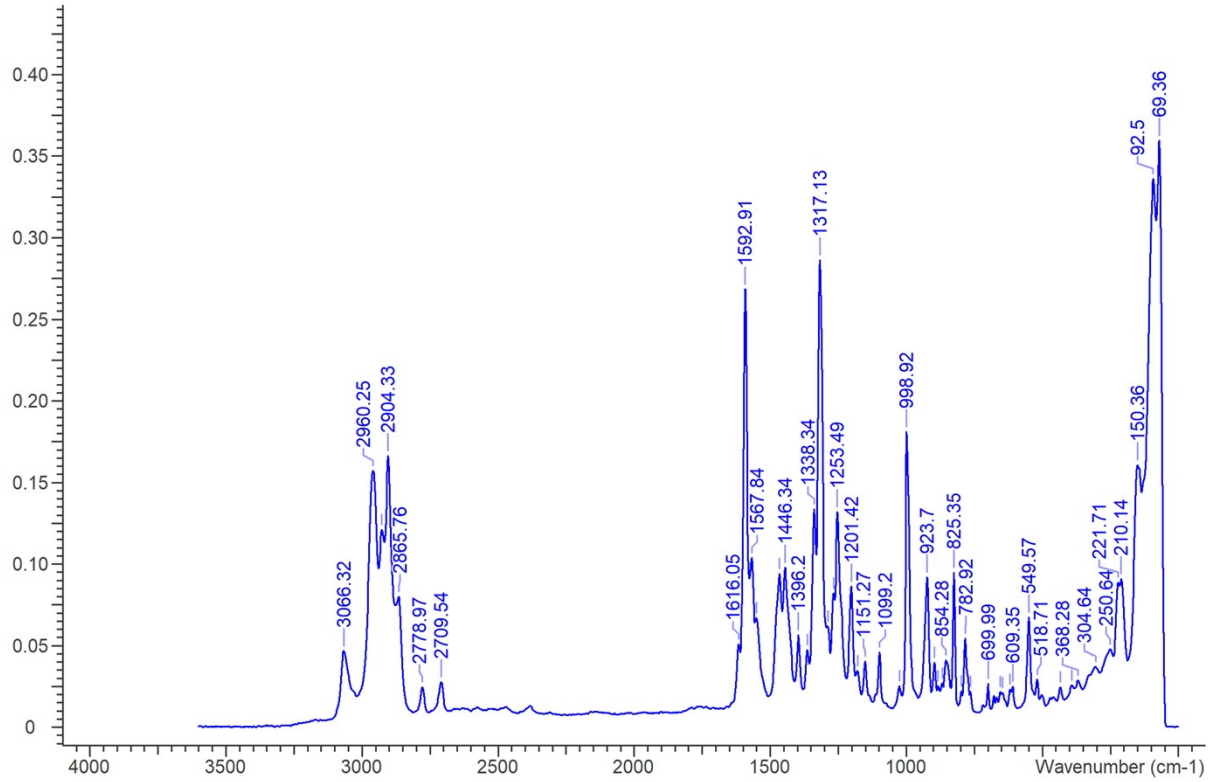


Figure S12: Raman spectrum of **3Ca·C_6H_6**.

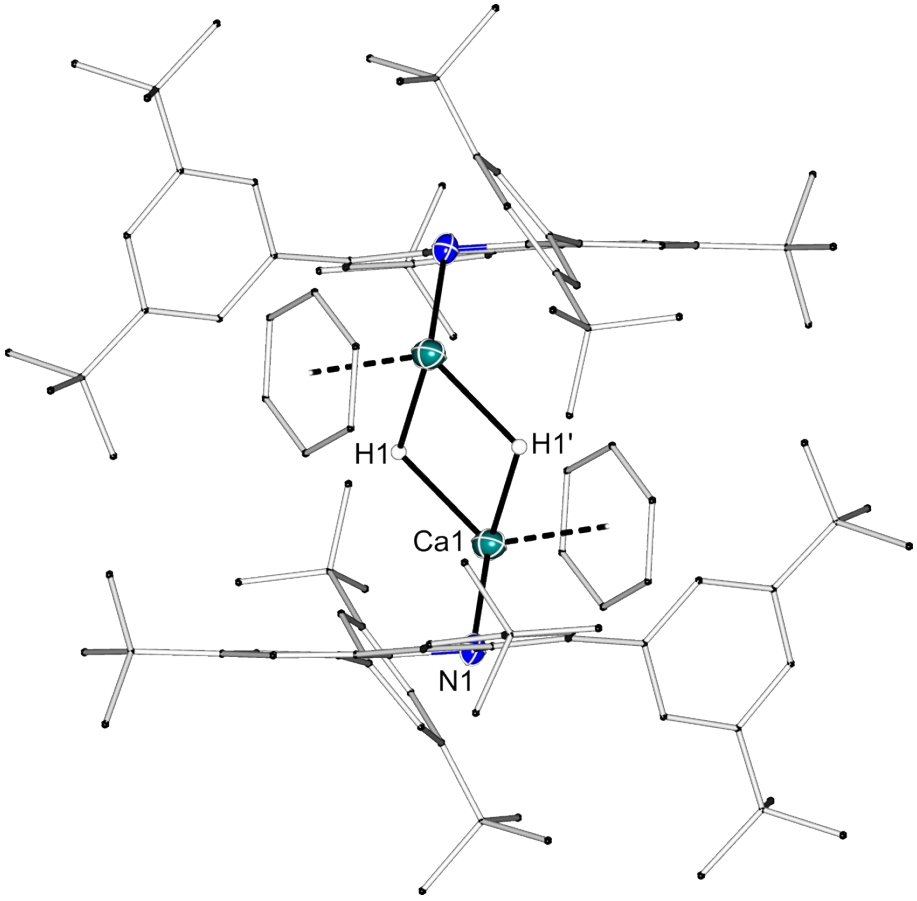


Figure S13: Molecular structure of **3Ca·C_6H_6**.

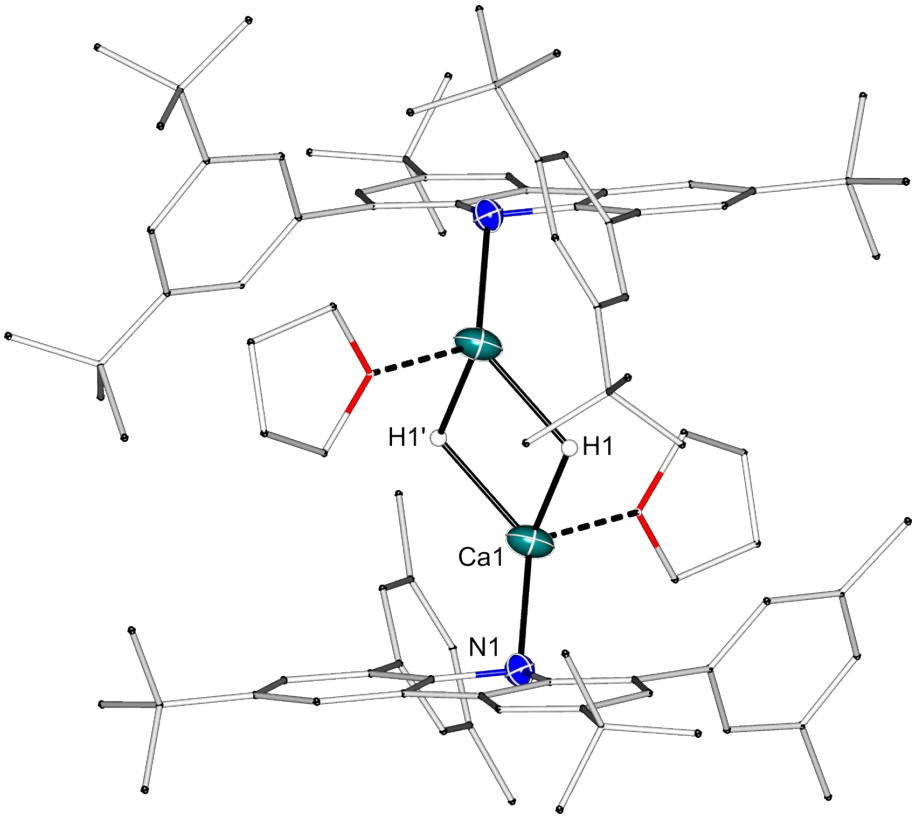
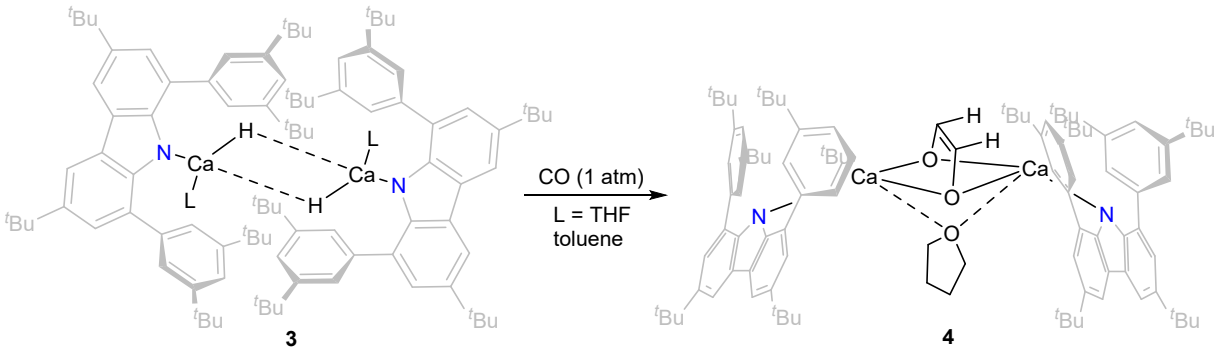


Figure S14: Molecular structure of **3Ca·THF**.

2.4 [(^{dtbp}Cbz)Ca(THF)COH]$_2$ (**4Ca**)



The calcium hydride **3Ca·THF** (94 mg, 0.068 mmol) was suspended in 1.1 mL C_6D_6, the corresponding suspension degassed and afterwards exposed to a carbon monoxide atmosphere. Within some minutes, the suspension turned bright orange and the consumption of the hydride **3Ca** is observed by a reduction of the yellow precipitate. The product crystallized from the reaction mixture. The solution phase was used for NMR characterization.

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.35 (br, s, 36 H, Ar-C(C*H*$_3$)$_3$), 1.51 (s, 18 H, Carb-C(C*H*$_3$)$_3$), 2.39 (br, s, 1 H, OC*H*), 7.46 (br, s, 2 H, *p*-C*H*), 7.49 (d, 2 H, $^4J_{HH}$ = 1.9 Hz, C^{2,7}*H*), 7.85 (br, s, 4 H, *o*-C*H*), 8.45 (d, 2 H, $^4J_{HH}$ = 1.9 Hz, C^{4,5}*H*).

^{13}C{^{1}H} NMR (100.7 MHz, C_6D_6): δ (ppm) = 31.95 (s, Ar-C(*C*H$_3$)$_3$), 32.59 (s, Carb-C(*C*H$_3$)$_3$), 34.75 (s, Carb-*C*(CH$_3$)$_3$), 35.24 (s, Ar-*C*(CH$_3$)$_3$), 69.46 (s, O*C*(H)) 115.91 (s, *C*H), 121.83 (s, *C*H), 123.82 (s, *C*H), 124.36 (s, *C*H), 127.29 (s), 132.00 (s), 138.81 (s), 142.73 (s), 147.47 (s), 152.29 (s).

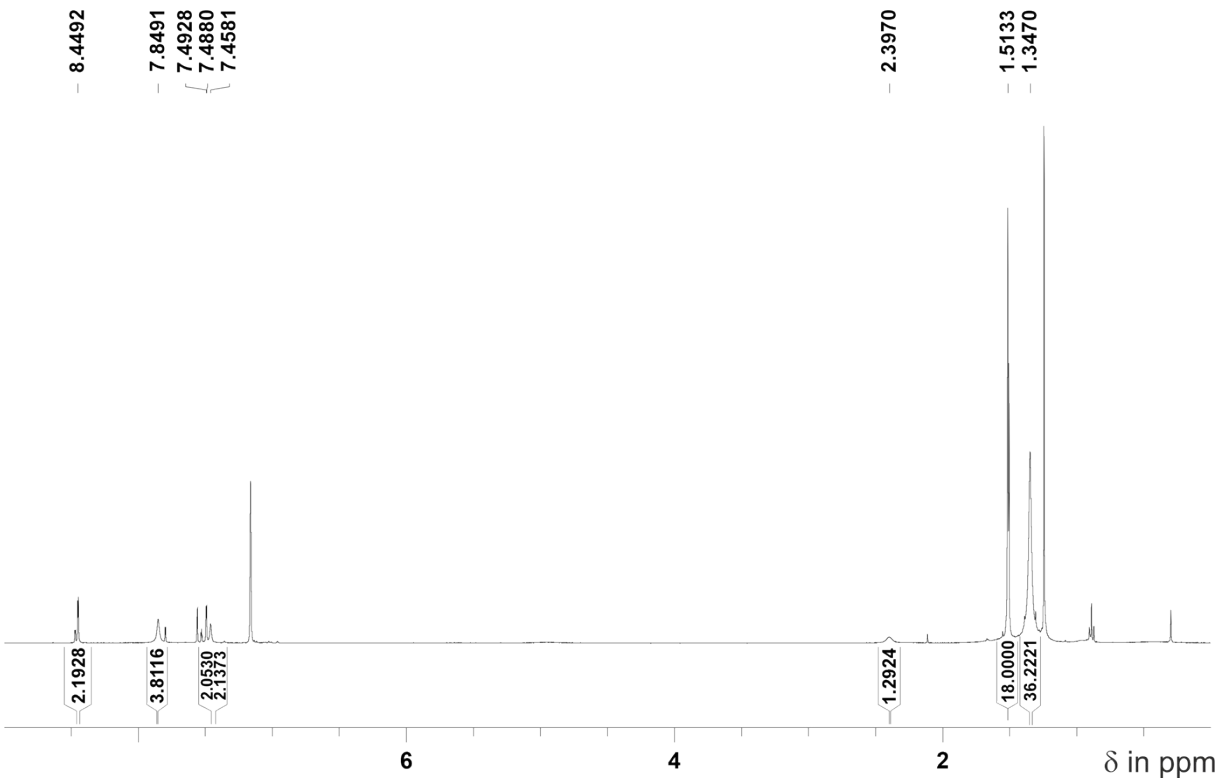


Figure S15: ^{1}H NMR spectrum of **4Ca**, unlabeled resonances are due to Cbz-H.

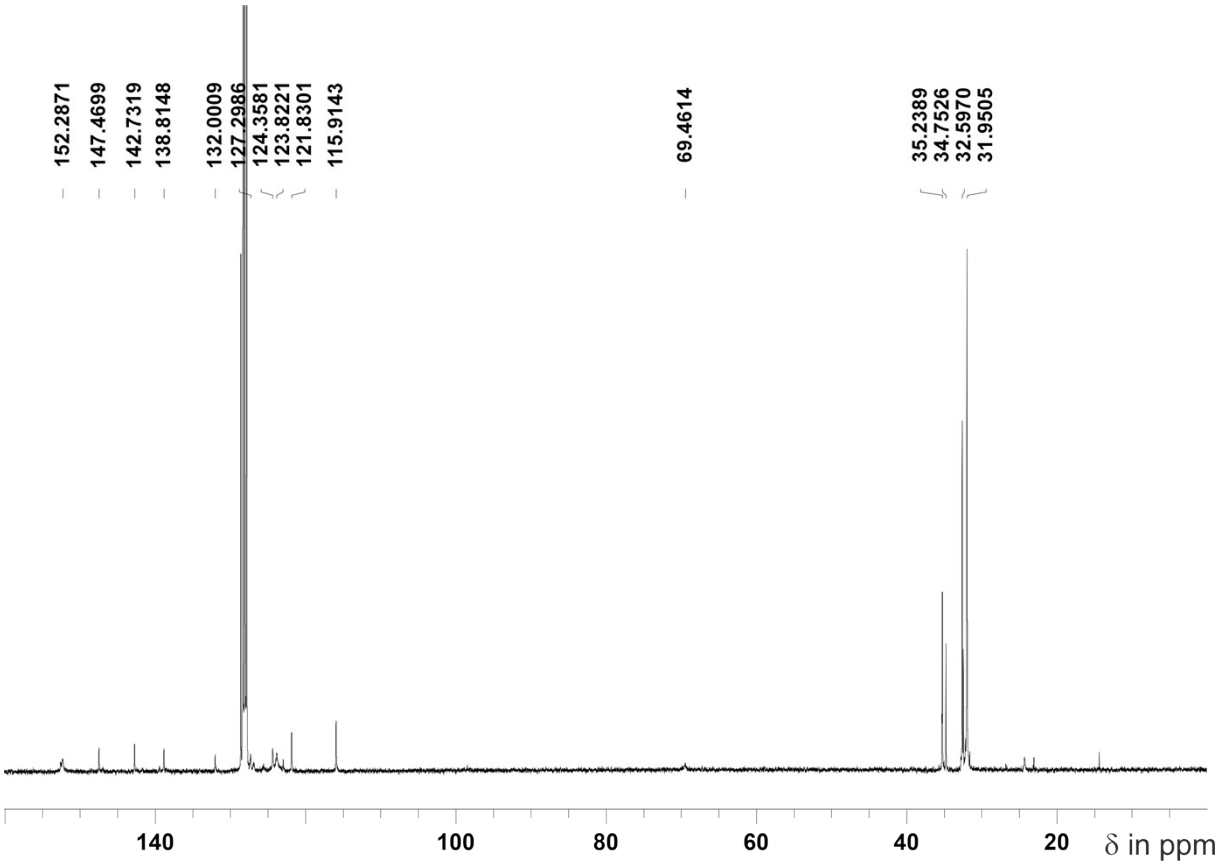


Figure S16: $^{13}C\{^{1}H\}$ NMR spectrum of **4Ca**.

2.5 [(^{dtbp}Cbz)Yb(SiMe$_3$)$_2$(THF)] (**1Yb**)

In a Schlenk flask, Yb(N{SiMe$_3$}$_2$)$_2$(THF)$_2$ (800 mg, 1.25 mmol) and ^{dtbp}CbzH (846 mg, 1.29 mmol) were combined as solids. Toluene (approx. 20 ml) were added via cannula and the mixture was stirred overnight. Afterwards, volatiles were removed in vacuo, affording an orange solid. The solid was washed with a small amount of *n*-hexane (2x 1 ml) and then dried again to yield [(^{dtbp}Cbz)YbN(SiMe$_3$)$_2$(THF)] (1160 mg, 1.09 mmol, 87%).

^{1}H NMR (C_6D_6): -0.17 (s, 18 H, Si*Me*$_3$), 1.06 (s, 4 H, OCH$_2$C*H*$_2$), 1.39 (s, 36 H, Ar-^{t}Bu), 1.54 (s, 18 H, Cbz-^{t}Bu), 2.93 (s, 4 H, OC*H*$_2$), 7.59 (s, 2 H, *p*-C*H*), 7.69 (s, 4 H, *o*-C*H*), 8.08 (s, 2 H, C^{2,7}*H*), 8.57 (s, 2 H, C^{4,5}*H*). **^{13}C NMR** (C_6D_6): 4.74 (s, J_{CSi} = 52.7 Hz, Si*C*), 24.59 (s, OCH$_2$*C*H$_2$), 31.55 (s, Ar-C(*C*H$_3$)$_3$), 32.12 (s, Cbz-C(*C*H$_3$)$_3$, 34.42 (s, Cbz-*C*(CH$_3$)$_3$, 34.97 (s, Ar-*C*(CH$_3$)$_3$, 68.89 (s, O*C*H$_2$CH$_2$), 115.96 (s, *C*H), 122.62 (s, *C*H), 123.26 (s, *o*-*C*H), 124.43 (s, *C*H), 126.42 (s), 127.98 (s, *C*$_6$H$_6$), 138.99 (s), 142.87 (s), 147.07 (s), 152.43 (s). **^{29}Si NMR** (C_6D_6): –16.2 (s). **^{171}Yb NMR** (C_6D_6): 668.8 (s).

IR (ATR, cm^{-1}): 378 (m), 403 (w), 410 (w), 422 (w), 435 (w), 455 (w), 462 (w), 475 (w), 502 (w), 520 (w), 549 (w), 584 (m), 605 (w), 619 (w), 646 (m), 666 (m), 697 (m), 719 (m), 746 (m), 763 (m), 781 (w), 811 (vs), 826 (vs), 843 (m), 856 (m), 867 (vs), 897 (w), 926 (w), 980 (w), 1026 (m), 1065 (s), 1150 (w), 1181 (w), 1202 (w), 1230 (vs), 1266 (m), 1284 (m), 1308 (w), 1337 (w), 1362 (m), 1379 (w), 1391 (m), 1433 (w), 1463 (m), 1476 (w), 1588 (w), 2869 (w), 2903 (m), 2956 (m).

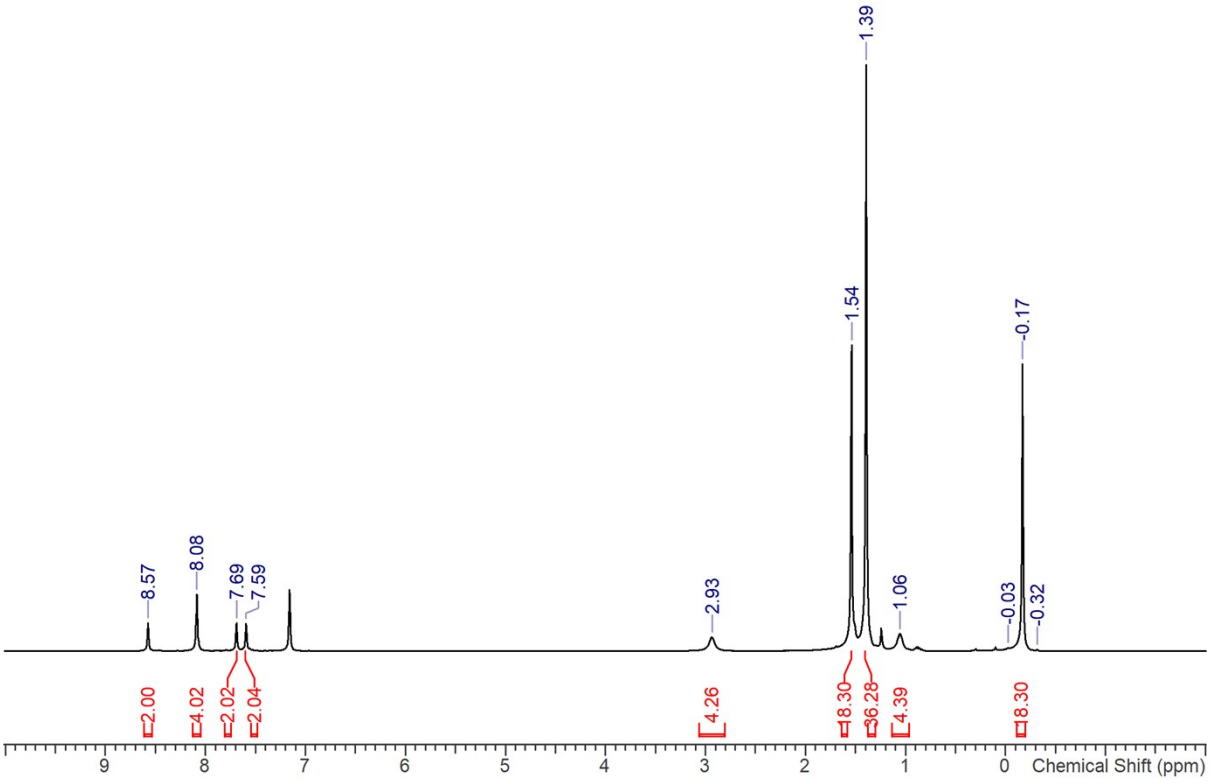


Figure S17: ^{1}H NMR spectrum of **1Yb**.

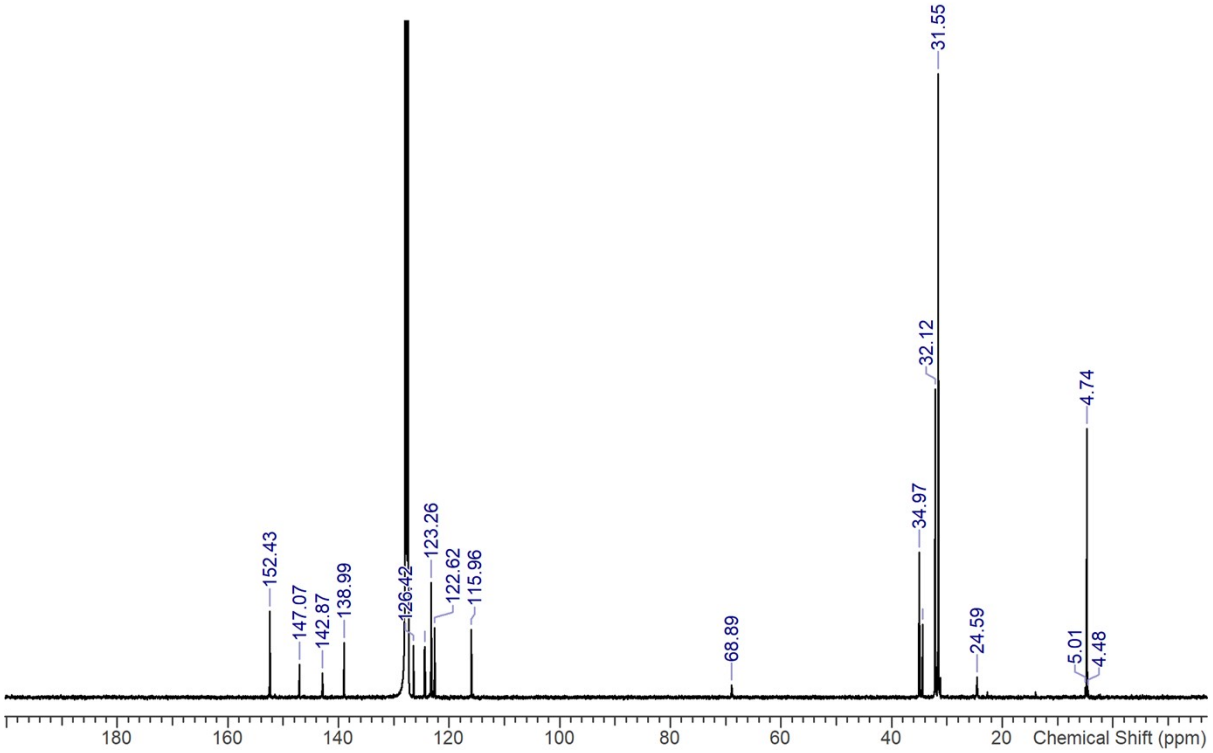


Figure S18: $^{13}C\{^{1}H\}$ NMR spectrum of **1Yb**.

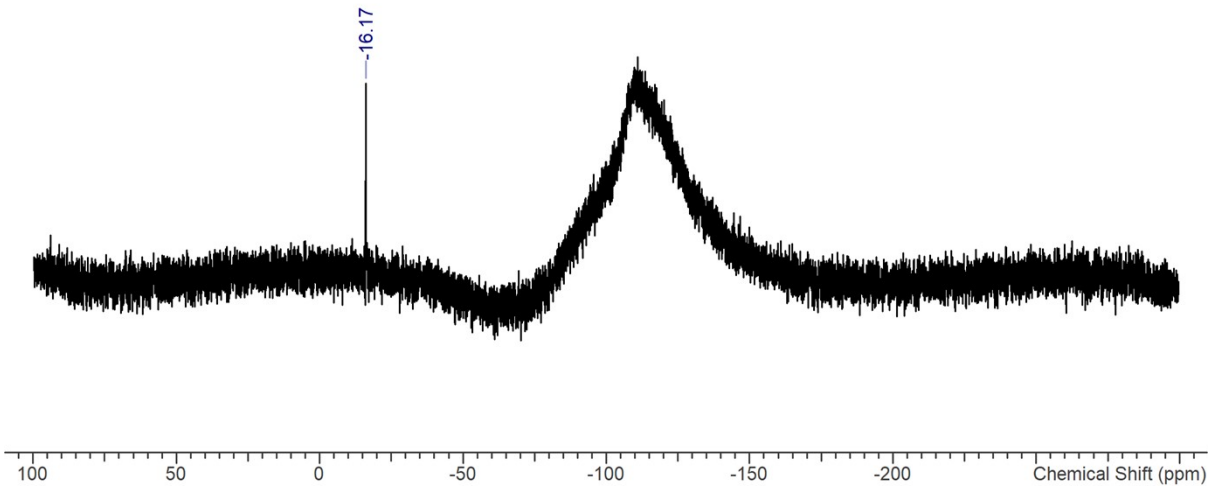


Figure S19: $^{29}Si\{^{1}H\}$ NMR spectrum of **1Yb**.

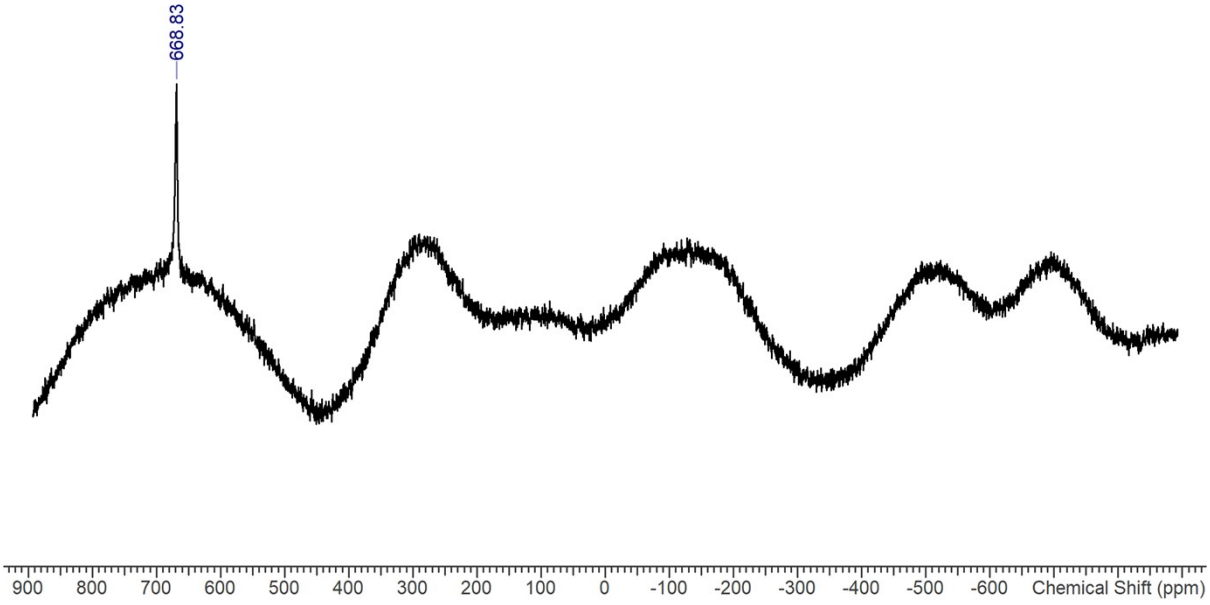


Figure S20: ^{171}Yb NMR spectrum of **1Yb**.

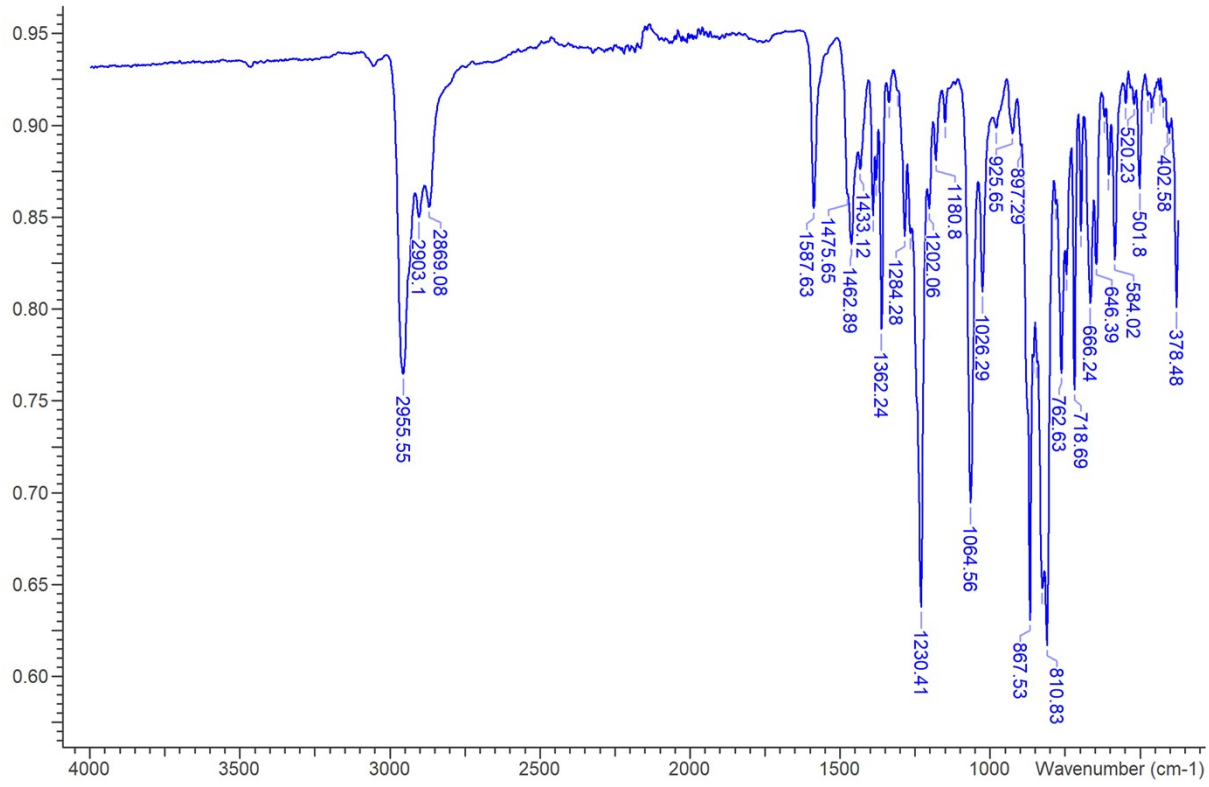


Figure S21: IR spectrum of **1Yb**.

2.6 [(^{dtbp}Cbz)Yb(C_6H_6)H] (**3Yb**·C_6H_6)

To 250 mg (0.236 mmol) [(^{dtbp}Cbz)Yb($SiMe_3$)$_2$(THF)], 5 ml of Et_2O were added. After dissolution, volatiles were evaporated in vacuo, then the sample was heated to 80 °C for 1 hour under dynamic vacuum. The process was repeated a second time. Then, the residue was dissolved in 3 ml of benzene and 50 mg of phenyl silane were added via microsyringe which immediately darkened the reaction mixture. The solution was left undisturbed overnight, depositing dark orange crystals of [(^{dtbp}Cbz)YbH(C_6H_6)]$_2$. The supernatant was removed via syringe and the crystals were washed with n-hexane (2x 1 ml). The crystals were then dried in vacuo for 30 minutes, affording [(^{dtbp}Cbz)YbH(C_6H_6)]$_2$ (46 mg, 0.025 mmol, 21%).

[(^{dtbp}Cbz)YbH(C_6H_6)]$_2$ was obtained when [(^{dtbp}Cbz)Yb($SiMe_3$)$_2$(THF)] with phenyl silane in *n*-hexane solution according to the above protocol.

NMR data could not be obtained due to insolubility of the compound.

IR (ATR, cm^{-1}): 388 (w), 398 (w), 411 (w), 424 (w), 438 (w), 462 (w), 473 (w), 500 (m), **550 (s)**, 618 (w), 642 (m), 676 (w), 699 (s), 707 (vs), 714 (s), 774 (m), **797 (m)**, 824 (w), 846 (s), 866 (s), 900 (w), 934 (w), 979 (w), 1028 (w), **1073 (s)**, 1151 (w), 1182 (w), 1202 (m), 1232 (vs), 1245 (s), 1267 (m), 1286 (m), 1340 (w), 1361 (s), 1381 (m), 1392 (m), 1433 (w), 1461 (m), 1473 (m), 1589 (m), 2866 (m), 2903 (m), 2954 (s), 3059 (vw).

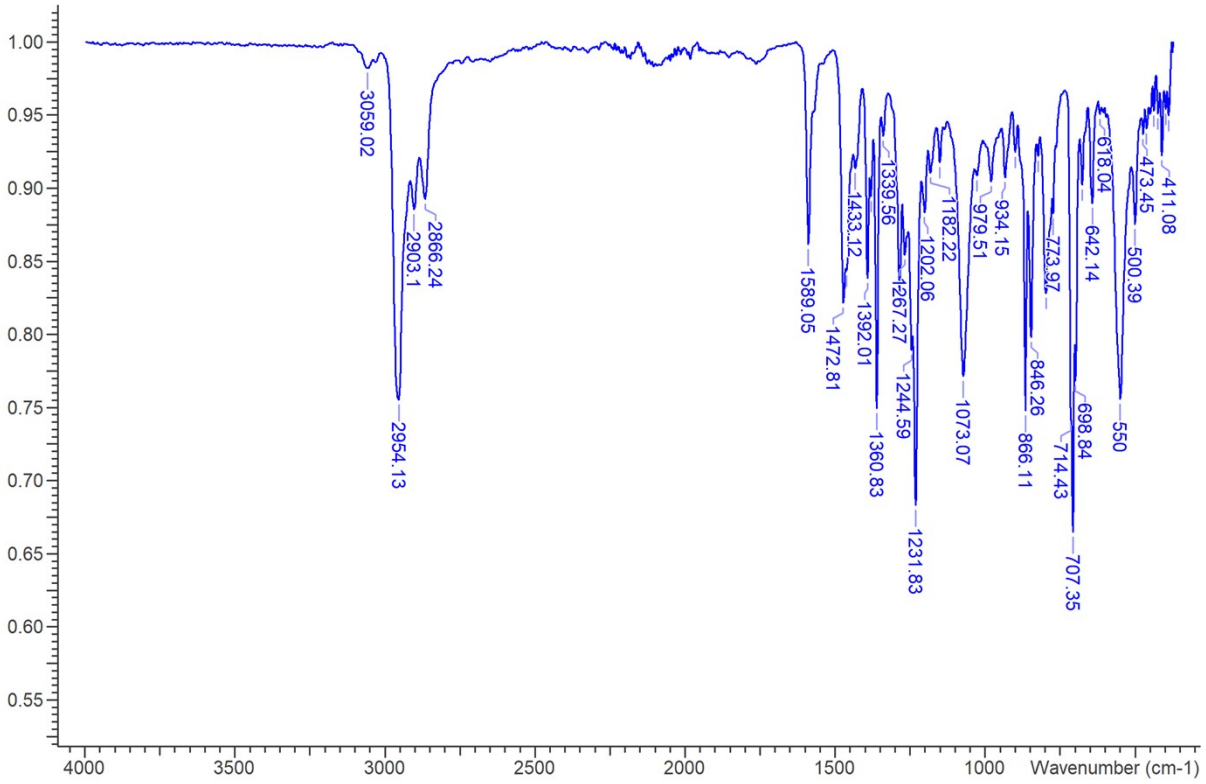


Figure S22: IR spectrum of **3Yb**·C_6H_6.

2.7 $[(^{dtbp}Cbz)_2Yb_2L_2(H_2C_2O_2)]$ (**4Yb**)

In a Young tube, 40 mg (22 µmol) of $[(^{dtbp}Cbz)Yb(L)_2H]_2$ were suspended in 2 ml of benzene. The suspension was degassed and then exposed to 1 bar of CO at ambient temperature. The solution phase darkened rapidly. After standing overnight, a small crop of new crystals formed that could be identified as the ethenediolate complex $[(^{dtbp}Cbz)_2Yb_2L_2(H_2C_2O_2)]$. The supernatant was evaporated solid was washed with 0.5 ml of *n*-hexane, affording $[(^{dtbp}Cbz)_2Yb_2L_2(H_2C_2O_2)]$ as orange solid (8 mg, 4 µmol, 19%). Redissolution in C_6D_6 did not allow NMR characterisation, as paramagnetic species formed.

IR (ATR, cm^{-1}): 386 (m), 394 (m), 404 (m), 414(m), 424 (m), 432 (m), 444 (m), 452 (m), 462 (m), 472 (m), 482 (w), 499 (m), 512 (w), 519 (m), 645 (m), 678 (m), 699 (s), 717 (s), 761 (m), 774 (m), 822 (s), 849 (s), 865 (s), 899 (m), 930 (s), 951 (m), 981 (m), 998 (w), 1016 (m), 1028 (m), 1070 (m), 1114 (m), 1134 (m), 1151 (m), 1184 (m), 1202 (m), 1208 (m), 1233 (s), 1245 (s), 1270 (s), 1284 (s), 1361 (s), 1392 (m), 1429 (m), 1461 (m), 1474 (m), 1589 (m), 2866 (m), 2903 (m), 2954 (s).

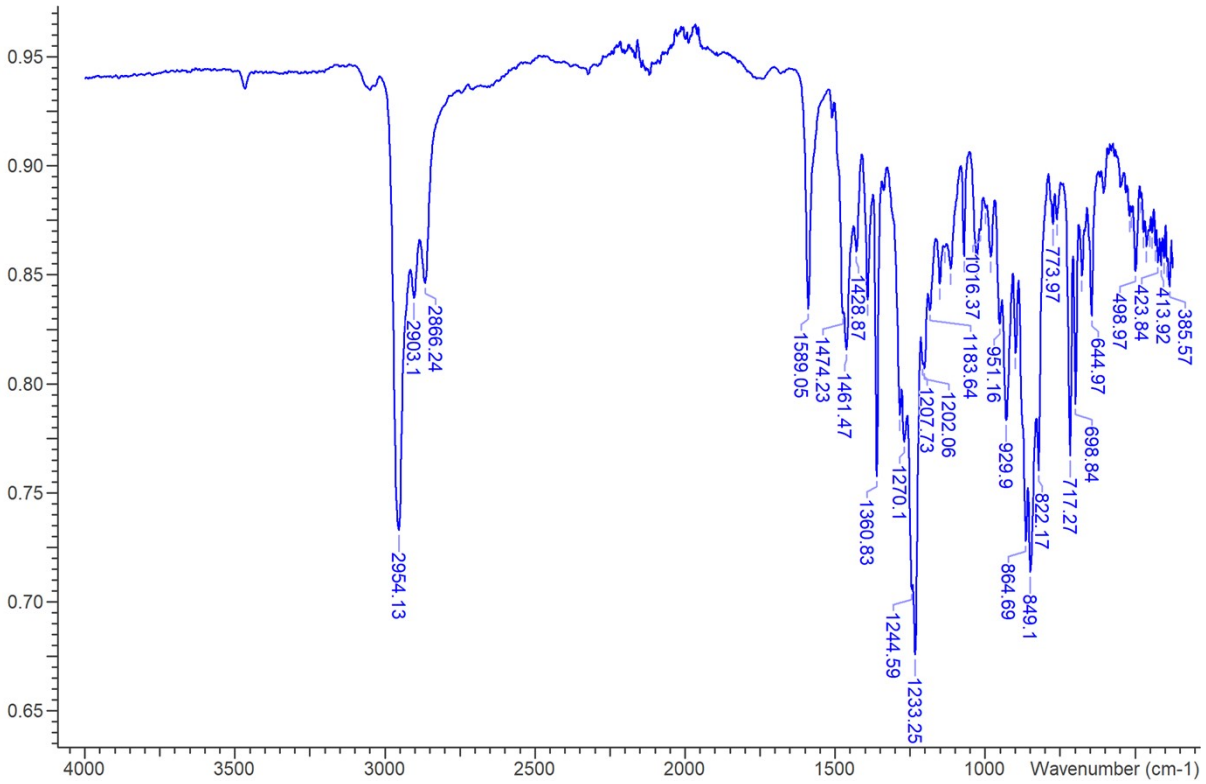


Figure S23: IR spectrum of **4Yb**.

2.8 [(^{dtbp}Cbz)CaD] (**3Ca-D·C_6H_6**)

The amide **2Ca** (138 mg, 0.161 mmol) was dissolved in 1.0 mL of benzene. To that solution, phenylsilane-d_3 (40 µL, 0.316 mmol, 1.96 eq.) was added via microsyringe. The mixture was shaken and then left undisturbed overnight. Afterwards, very small crystals were observed. The solution was concentrated to half of its volume and left undisturbed for at least five hours. Crystalline material formed. The supernatant was removed, the crystals were washed multiple times with *n*-hexane and briefly dried. The characterisation data were obtained from the crystalline material.

IR (ATR) ũ (cm^{-1}) = 388 (s), **404 (s),** 456 (vw), 499 (w), 519 (w), 547 (w), 556 (w), **571 (w),** 602 (w), 617 (w), 646 (m), 676 (m), 699 (m), 716 (m), **774 (m),** 825 (w), 848 (m), 865 (s), 899 (w), 921 (w), 931 (w), 980 (vw), 1026 (w), 1072 (vw), 1150 (w), 1184 (w), 1201 (w), 1232 (vs), 1245 (s), 1269 (m), 1284 (m), 1338 (w), 1361 (s), 1382 (w), 1392 (m), 1430 (w), 1466 (m), 1569 (w), 1589 (m), 2865 (m), 2902 (m), 2954 (s).

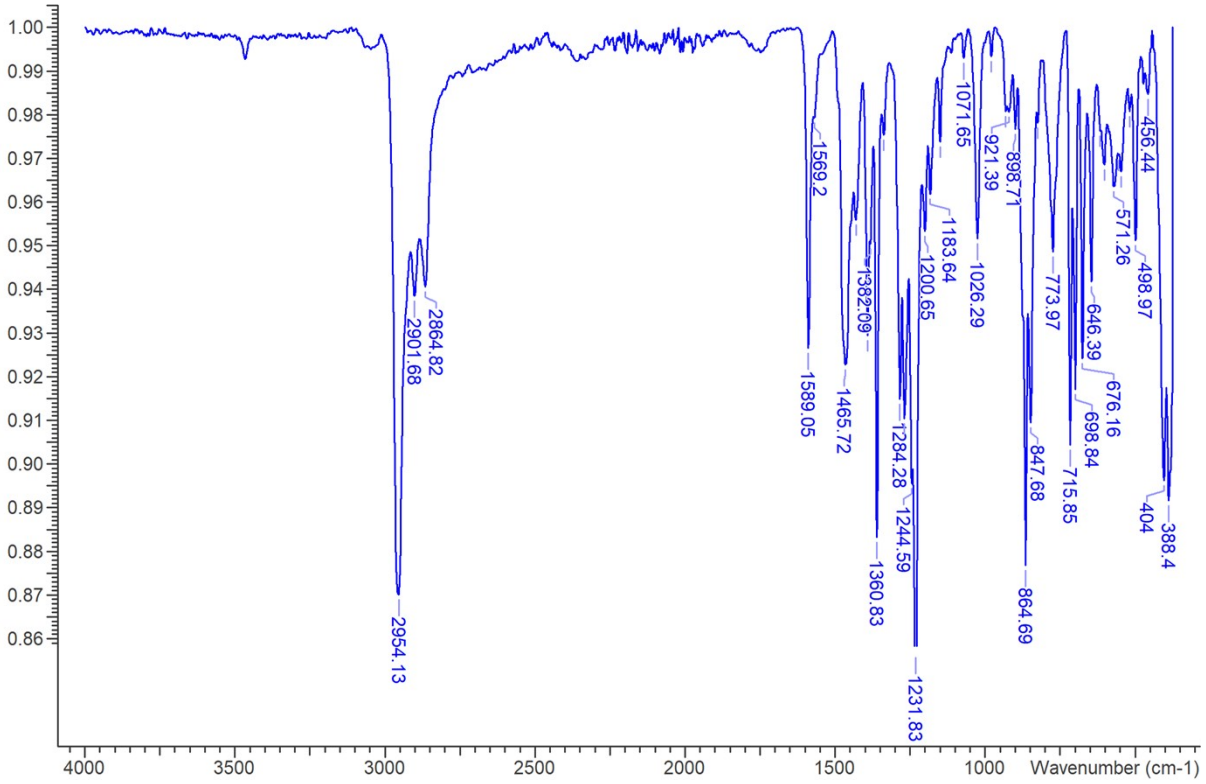


Figure S24: IR spectrum of **3Ca-D·C_6H_6**.

3 Crystallographic Details

Table S1: Crystallographic details for **1Ca** and **2Ca**.

	$RCaN(SiMe_3)_2(THF)$ (**1Ca**)	$RCaN(SiMe_3)_2(THF)$ (**1Ca** hexane solvate)	$RCaN(SiMe_3)_2$ (**2Ca**)
CCDC #	2145430	2145431	2145432
Empirical formula	$C_{58}H_{90}N_2OSi_2Ca$	$C_{61}H_{97}N_2OSi_2Ca$	$C_{54}H_{82}N_2Si_2Ca$
FW [g mol^{-1}]	927.57	970.66	855.47
Wavelength [Å]	0.71073	0.71073	0.71073
Temperature [K]	200(2)	200(2)	200(2)
Crystal system	monoclinic	triclinic	monoclinic
Space group	$P2_1/n$	P-1	$P2_1/n$
a [Å]	16.1404(4)	11.859(3)	16.4998(8)
b [Å]	18.4014(3)	14.163(2)	16.2635(10)
c [Å]	19.6125(5)	18.825(3)	20.1945(10)
α [°]	90	92.034(11)	90
β [°]	97.612(2)	106.542(14)	91.354(4)
γ [°]	90	92.672(15)	90
V [Å^3]	5773.7(2)	3023.7(9)	5417.6(5)
Z	4	2	4
ρ_{calc} *(g·cm^{-3})*	1.067	1.066	1.049
μ	0.187	0.181	0.194
F(000)	2032	1066	1872
reflections collected	51714	37684	36337
independent reflections	15576	37684	14389
reflectionsGT (I > 2σ(I))	11636	27827	10093
R_{int}	0.0238	0.0228	0.0312
parameters	737	769	793
restraints	690	762	1321
GooF	1.025	1.026	1.035
R1	0.0459	0.0487	0.0497
R1 (all)	0.0675	0.0719	0.0756
wR2	0.1162	0.1275	0.1292
wR2 (all)	0.1311	0.1436	0.1465
weight factors	0.0629 1.7805	0.0692 0.8587	0.0705 1.2183

Table S2: Crystallographic details for **2Ca** (dimer), and **3Ca**.

	RCaH·THF (**3Ca**·THF)	RCaH·C_6H_6 (**3Ca**·C_6H_6)	$[RCa(OCH)]_2$·THF (**4Ca**)
CCDC #	2145437	2145438	2372502
Empirical formula	$C_{52}H_{73}NOCa$	$C_{66}H_{83}NCa$	$C_{102}H_{138}Ca_2N_2O_3$
FW [g mol^{-1}]	768.19	930.41	1520.30
Wavelength [Å]	0.71073	1.34143	1.34143
Temperature [K]	200(2)	150(2)	180(2)
Crystal system	triclinic	triclinic	monoclinic
Space group	*P*-1	*P*-1	*C*2/*c*
a [Å]	13.1101(5)	13.7368(8)	17.5438(5)
b [Å]	13.6268(5)	16.0770(8)	21.5053(4)
c [Å]	14.1886(6)	16.7076(11)	26.0497(7)
α [°]	74.213(3)	103.641(4)	90
β [°]	86.447(3)	110.348(5)	106.954(2)
γ [°]	76.820(3)	113.208(4)	90
V [Å^3]	2374.91(17)	2866.6(3)	9401.0(4)
Z	2	2	4
ρ_{calc} (g·cm^{-3})	1.074	1.078	1.074
μ	0.167	0.800	0.926
F(000)	840	1012	3312
reflections collected	21167	35762	31824
independent reflections	10846	13326	10346
reflectionsGT (I > 2σ(I))	7775	10810	7308
R_{int}	0.0243	0.0160	0.0249
parameters	692	813	578
restraints	985	1381	330
GooF	1.063	1.098	1.111
R1	0.0554	0.0508	0.0478
R1 (all)	0.0864	0.0603	0.0688
wR2	0.1260	0.1521	0.1338
wR2 (all)	0.1450	0.1578	0.1411
weight factors	0.0538 1.4404	0.0971 0.4752	0.0788 0.6480

Table S3: Crystallographic details for **1Yb**, **2Yb** and **3Yb**.

	$RYbNT_2 \cdot THF$ (**1Yb**)	$RYbH \cdot THF$ (**3Yb**·THF)	$RYbH \cdot C_6H_6$ (**3Yb**·C_6H_6)	$[RYb(OCH)]_2$ (**4Yb**)
CCDC #	2372499	2372500	2372501	2372503
Empirical formula	$C_{61}H_{97}N_2OSi_2Yb$	$C_{52}H_{73}NOYb$	$C_{66}H_{83}NYb$	$C_{113.33}H_{150.67}N_2O_{3.33}Yb_2$
FW [g mol⁻¹]	1103.62	901.15	1063.37	1940.43
Wavelength [Å]	1.34143	0.71073	0.71073	0.71073
Temperature [K]	150(2)	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	triclinic	triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1
a [Å]	11.7801(6)	12.930(2)	13.6301(5)	14.3009(8)
b [Å]	14.1233(8)	13.419(2)	16.0796(5)	21.2924(11)
c [Å]	18.7536(10)	13.9153(19)	16.2110(5)	27.1108(13)
α [°]	92.001(4)	74.266(12)	114.438(2)	66.923(4)
β [°]	106.563(4)	86.131(12)	95.447(3)	84.961(4)
γ [°]	92.221(4)	76.624(13)	113.394(3)	85.933(4)
V [Å³]	2985.0(3)	2260.9(6)	2822.27(18)	7559.3(7)
Z	2	2	2	3
ρ_{calc} *(g·cm⁻³)*	1.228	1.324	1.251	1.279
μ	5.583	2.105	1.696	1.895
F(000)	1166	940	1112	3034
reflections collected	34055	20802	29707	101366
independent reflections	12109	8751	12569	29716
reflectionsGT (I > 2σ(I))	6793	6221	11112	13919
R_{int}	0.0928	0.0792	0.0242	0.1144
parameters	648	548	813	2239
restraints	100	162	1381	2783
GooF	0.831	1.078	1.098	1.000
R1	0.0502	0.0623	0.0302	0.0819
R1 (all)	0.1011	0.1035	0.0376	0.1873
wR2	0.0985	0.1334	0.0744	0.1881
wR2 (all)	0.1095	0.1695	0.0768	0.2462
weight factors	0.0488 0	0.0536 22.4962	0.0477 1.8778	0.1263 0

4 Computational Details

All computations were performed using Gaussian16[10] utilizing the PBE1PBE level of theory, Def2SVP basis sets and empirical dispersion correction (GD3). Yb was included with a large ECP (ECP60MDF) and corresponding basis set.[11] No solvent corrections were applied. All optimized molecular structures where checked to be minima on the energy hypersurface and possess no imaginary vibrational frequencies.

4.1 Vibrational modes in **3Ca**·C_6H_6 and **3Yb**·C_6H_6

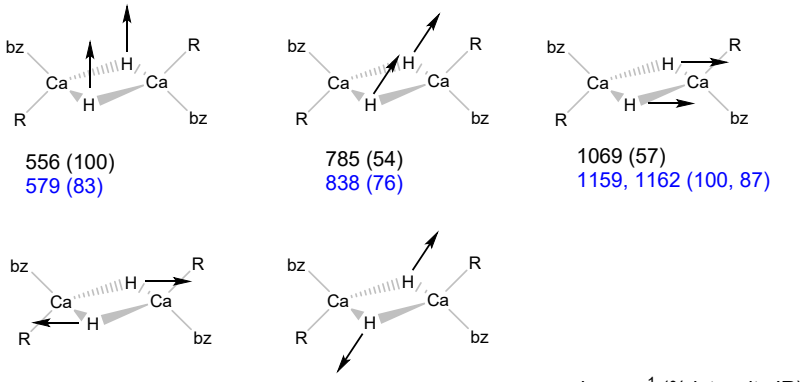


Figure S25: Observed vs. (unscaled) calculated vibrational data for the hydride-involving vibrational modes for **3Ca**·C_6H_6.

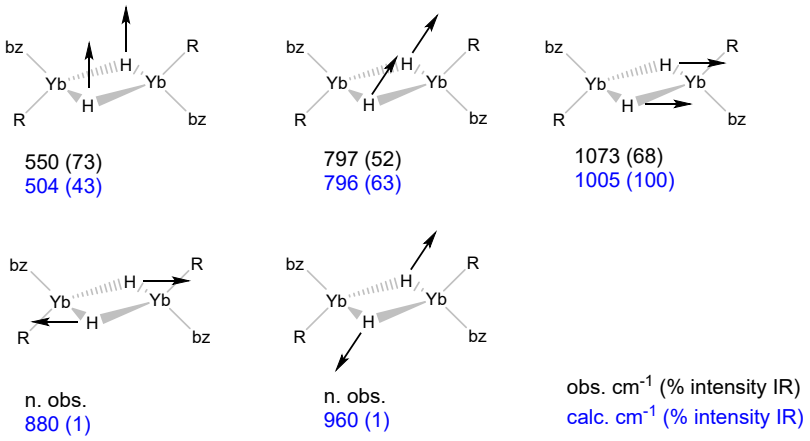


Figure S26: Observed vs. (unscaled) calculated vibrational data for the hydride-involving vibrational modes for **3Yb**·C_6H_6.

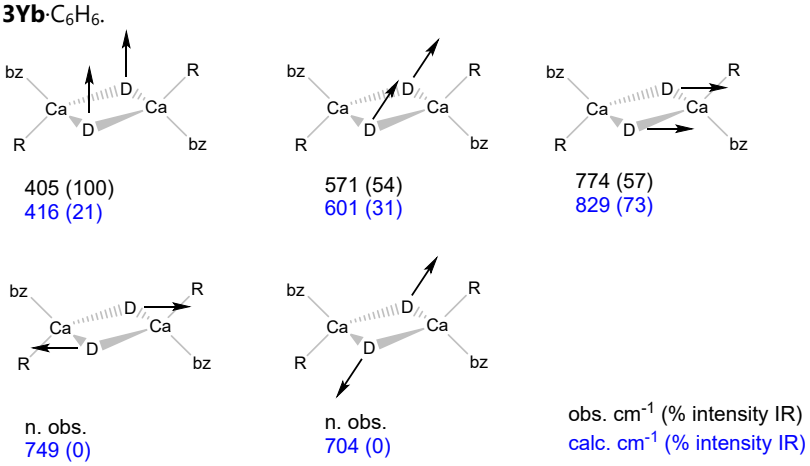


Figure S27: Observed vs. (unscaled) calculated vibrational data for the hydride-involving vibrational modes for **3Ca-D**·C_6H_6.

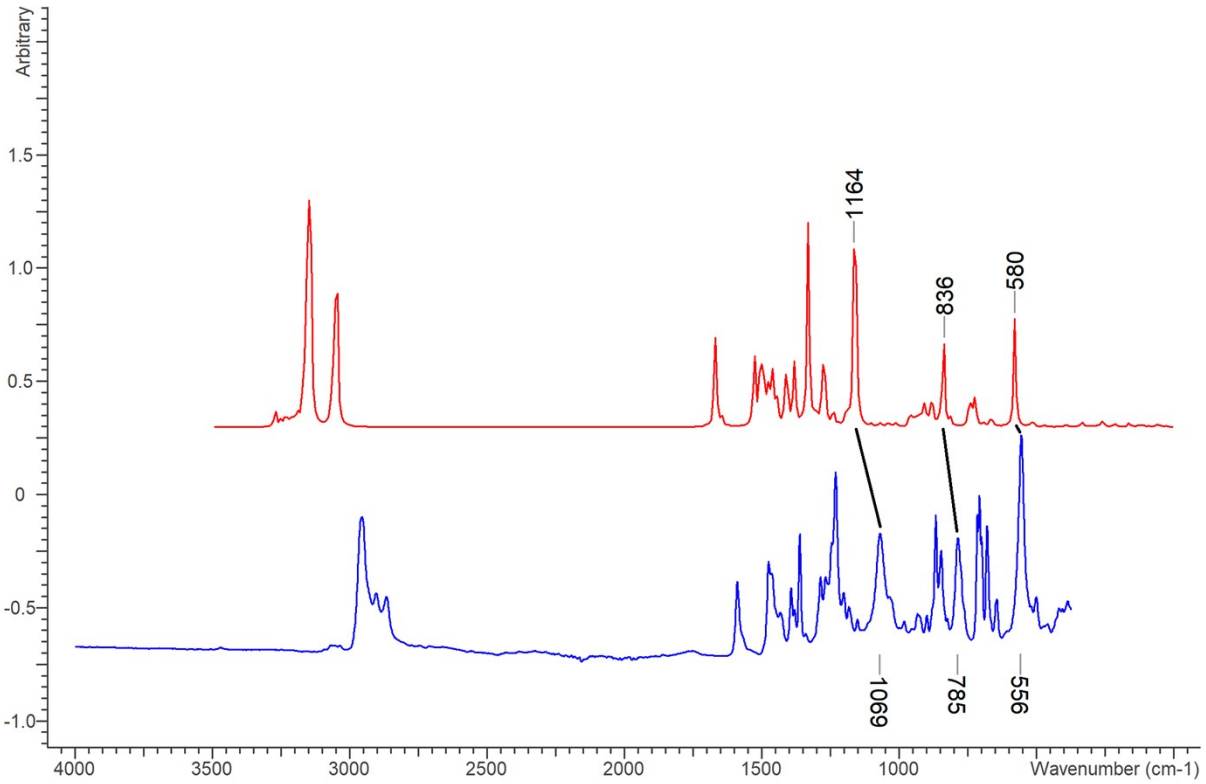


Figure S28: Unscaled computed (red) and observed (blue) IR spectrum **3Ca**·bz. Hydride-involving bands are marked.

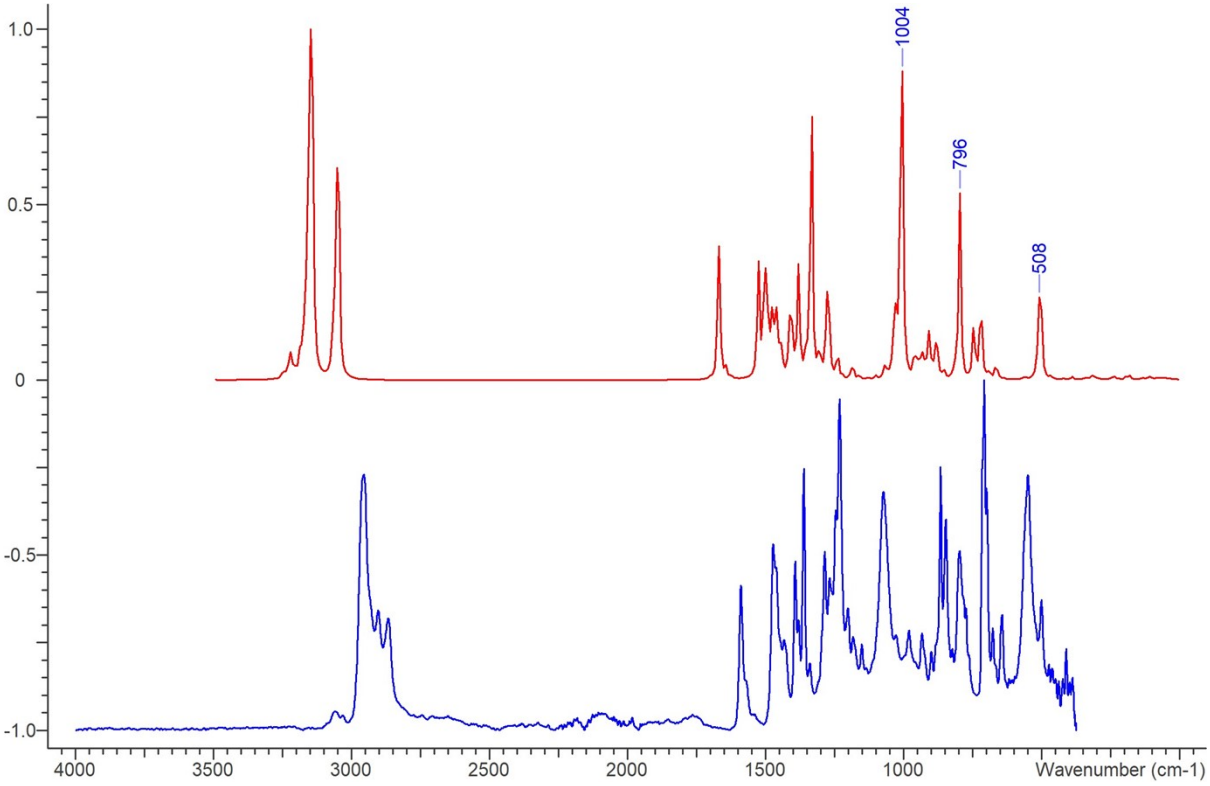


Figure S29: Unscaled computed (red) and observed (blue) IR spectrum **3Yb**·bz. Hydride-involving bands are marked.

4.2 Optimised Structures

4.2.1 (^{dtbp}Cbz)CaN(SiMe$_3$)$_2$

0 1

Ca	0.24884900	-0.91894500	0.08150300
Si	-0.15506300	-3.39253300	-1.86256800
Si	-0.52017100	-0.69214400	-3.32455800
C	-1.09331100	1.00286700	-2.72308500
H	-1.34385700	1.65850100	-3.57257400
H	-0.31461600	1.51733300	-2.13466300
H	-1.98694200	0.92867600	-2.08265400
C	0.97090500	-0.39923500	-4.45229000
H	1.37820500	-1.34622700	-4.84147000
H	1.77798500	0.11646900	-3.90829400
H	0.69251000	0.22913900	-5.31430100
C	-1.88071200	-1.42989800	-4.41399300
H	-1.58464700	-2.41191700	-4.81880600
H	-2.09614300	-0.77017500	-5.27025500
H	-2.81430200	-1.56519600	-3.84783500
N	0.08259000	1.29325100	0.67506500
N	-0.13238200	-1.68492700	-1.96217100
C	-1.03095400	2.09740900	0.65318600
C	-2.38542900	1.70984500	0.68820000
C	-3.35298100	2.71354500	0.56604800
H	-4.39780700	2.40392200	0.61292100
C	-3.04228100	4.07798100	0.41789900
C	-1.69254400	4.44220100	0.37697900
H	-1.40619900	5.48952100	0.24608100
C	-0.69538400	3.47332100	0.48457500
C	0.74275800	3.50510300	0.39568600
C	1.68875600	4.51167200	0.17176800
H	1.34886500	5.54421400	0.07735000
C	3.04183200	4.19236600	0.05298100
C	3.41876300	2.83440600	0.17034800
H	4.47389200	2.56063300	0.08256500
C	2.50781600	1.81023400	0.41335700
C	1.14590100	2.14951100	0.52110900
C	-2.78935700	0.29403800	0.81325000
C	-2.18959900	-0.55376800	1.76857800
H	-1.43838100	-0.11282800	2.42869200
C	-2.64021100	-1.86647600	1.96412300
C	-3.68057700	-2.33688000	1.14761200
H	-4.04121700	-3.35294000	1.29501700
C	-4.29031000	-1.53375000	0.18050000
C	-3.82167300	-0.22333800	0.02468200
H	-4.27001200	0.43203500	-0.72494000
C	-2.14350900	-2.71474000	3.13980700
C	-0.74216800	-2.29328100	3.58345100
H	-0.38052200	-2.94702300	4.39110300
H	-0.71171700	-1.26159700	3.96154500
H	-0.01279100	-2.37603500	2.76032100
C	-2.11510100	-4.20995300	2.79648600
H	-3.12024300	-4.61115700	2.60437900
H	-1.69741100	-4.78081000	3.64009700
H	-1.49861400	-4.41587300	1.90879600
C	-3.11493700	-2.48988400	4.31163800
H	-4.13582800	-2.79586100	4.03748600
H	-3.14836700	-1.42738400	4.59688900
H	-2.80442100	-3.07580700	5.19202000
C	-5.46998300	-2.01895700	-0.66779500
C	-5.80828000	-3.48793100	-0.40406500
H	-6.11124700	-3.66002900	0.64033900
H	-4.95838900	-4.14890200	-0.63416500
H	-6.64915200	-3.79479100	-1.04437500
C	-6.70018800	-1.16438100	-0.32136700
H	-7.57135700	-1.49126600	-0.91139400
H	-6.52995900	-0.09895900	-0.53696600
H	-6.95502200	-1.25454800	0.74604400
C	-5.13787800	-1.86258100	-2.15819900
H	-5.99303100	-2.18190700	-2.77465000
H	-4.27070700	-2.48072100	-2.43026000
H	-4.90570400	-0.82131800	-2.42498900
C	-4.12502700	5.15730400	0.29487100
C	-5.53798800	4.57188600	0.35262600
H	-5.71838100	3.85848900	-0.46649500
H	-6.28087700	5.37918100	0.25828800

H	-5.72832800	4.05570700	1.30629600
C	-3.97647300	6.16449900	1.44561100
H	-4.74165800	6.95493400	1.37302400
H	-2.98995700	6.65153400	1.43447300
H	-4.08994800	5.66416500	2.41985300
C	-3.96511100	5.88703800	-1.04805800
H	-4.06690900	5.18382200	-1.88915300
H	-2.97993200	6.36889900	-1.13520000
H	-4.73227000	6.67106200	-1.15888300
C	4.12696100	5.24480600	-0.20070500
C	3.54309400	6.65445200	-0.31486900
H	2.82962500	6.73349100	-1.14947000
H	4.35049100	7.38058400	-0.49753800
H	3.02630900	6.95745400	0.60869100
C	5.13300300	5.23496200	0.96094200
H	5.61916700	4.25396700	1.07158000
H	4.63171500	5.46829300	1.91308400
H	5.92498600	5.98405100	0.79631100
C	4.85804900	4.92182000	-1.51339800
H	5.33963000	3.93288200	-1.48074300
H	5.64371700	5.66847000	-1.71481600
H	4.15617000	4.92382700	-2.36171800
C	2.94685200	0.39654700	0.52373300
C	3.50274300	-0.25979000	-0.57967400
H	3.55969600	0.28795900	-1.52156800
C	3.99151800	-1.57400200	-0.48431900
C	3.91570500	-2.20349400	0.75933500
H	4.31554000	-3.21224500	0.86238200
C	3.36551500	-1.58482700	1.89593700
C	2.84751300	-0.29245900	1.75105200
H	2.42163200	0.24481900	2.59960100
C	4.64734500	-2.24976400	-1.69064700
C	3.92432800	-1.85142600	-2.98289300
H	4.30701700	-2.44051100	-3.83033300
H	4.07721400	-0.79255400	-3.23559500
H	2.84052400	-2.01839400	-2.90330800
C	6.10990600	-1.78058000	-1.75592000
H	6.61895900	-2.22845100	-2.62457400
H	6.66066800	-2.06964600	-0.84723800
H	6.16976200	-0.68561400	-1.85265300
C	4.61738300	-3.77722300	-1.56797200
H	3.59070300	-4.15244000	-1.43776100
H	5.22691900	-4.14257900	-0.72784500
H	5.02755100	-4.23170600	-2.48230000
C	3.45164800	-2.30162800	3.24794600
C	4.93922200	-2.45207100	3.61119800
H	5.04471400	-2.94767600	4.58951400
H	5.43039000	-1.46874300	3.66999100
H	5.48206800	-3.05534000	2.86830700
C	2.81321500	-3.69555500	3.15711100
H	1.75042400	-3.63625700	2.88239300
H	2.88313800	-4.21001300	4.12839200
H	3.31276000	-4.33097100	2.41111400
C	2.76868400	-1.50939300	4.36431600
H	1.70538700	-1.32878200	4.15408700
H	3.25327100	-0.53496200	4.52633700
H	2.83005900	-2.06919300	5.30987900
C	0.60137100	-3.82034600	-0.14856800
H	1.62235000	-3.42199800	-0.00589400
H	0.68012900	-4.91199900	-0.02498700
H	-0.03449400	-3.49623400	0.69856500
C	0.84205000	-4.31646500	-3.17316700
H	0.80357300	-5.40608100	-3.01154200
H	1.89728200	-4.00738500	-3.19136700
H	0.42168700	-4.11330500	-4.17182000
C	-1.88307300	-4.15685100	-1.83940900
H	-2.38825700	-4.00402700	-2.80607300
H	-2.49714000	-3.67780800	-1.06036600
H	-1.85189100	-5.24106000	-1.64184400

4.2.2 [(^{dtbp}Cbz)CaN(SiMe$_3$)$_2$]$_2$

0 1

Ca	1.47046300	-0.70278600	-0.09608800
N	0.20829200	0.49483500	1.52553900
Si	-0.77384500	-0.71069300	2.33820200
C	-2.49808100	-0.05844500	2.73048100

H	-2.44170200	0.67340400	3.55019800
H	-3.12590400	-0.89608100	3.07282100
H	-3.06071400	0.40637800	1.90193900
C	-0.95264300	-2.12509700	1.09998700
H	-1.67434600	-2.84967500	1.49998100
H	-0.01304100	-2.68945500	0.96715600
H	-1.34922800	-1.82726500	0.11797400
C	-0.12120700	-1.47401700	3.92054400
H	-0.72354700	-2.37030500	4.13406100
H	-0.20868600	-0.80347300	4.78537300
H	0.92700500	-1.78964500	3.82142000
Si	0.85769600	1.80685200	2.50050700
C	1.51454800	1.33354600	4.20140700
H	2.07903400	2.19571700	4.59277800
H	2.21068600	0.48258800	4.14590700
H	0.72361200	1.09891400	4.92759500
C	2.32623800	2.62321900	1.66056700
H	2.62380900	3.51020000	2.24360300
H	2.17076300	2.94299500	0.62287500
H	3.17647700	1.92560900	1.68528700
C	-0.48903500	3.09884500	2.77477900
H	-0.12530300	3.91867900	3.41300200
H	-1.36190800	2.65611600	3.27564600
H	-0.85303000	3.57418300	1.84855800
N	3.63247200	-1.38864700	0.70162500
C	3.10418300	-2.47448000	1.37104900
C	2.33155800	-3.55357700	0.86394000
C	1.84804300	-4.49086400	1.79603100
H	1.29327900	-5.33762500	1.39390100
C	2.11061300	-4.45325800	3.17226800
C	2.92065200	-3.41524100	3.64625300
H	3.18822400	-3.35662400	4.70488600
C	3.39792600	-2.44498800	2.77093200
C	4.21319500	-1.27850200	2.95676700
C	4.77984300	-0.71554000	4.09904400
H	4.62648100	-1.20332900	5.06583000
C	5.52751400	0.45742200	4.00205100
C	5.70509700	1.00213800	2.71867700
H	6.33416100	1.88492200	2.60092900
C	5.16259200	0.46639200	1.54171000
C	4.35382900	-0.69173900	1.66090800
C	2.14578500	-3.86799000	-0.57781100
C	3.20446900	-3.70991300	-1.48261900
H	4.09220800	-3.17641800	-1.13771900
C	3.16059300	-4.28843800	-2.76017900
C	2.00750200	-4.98226700	-3.12948300
H	1.96298800	-5.44857900	-4.11320800
C	0.89418000	-5.10183700	-2.28332300
C	0.97906600	-4.52916900	-1.01606800
H	0.14657400	-4.62776700	-0.31931300
C	4.35953100	-4.14364200	-3.70208300
C	5.65190500	-4.52286000	-2.96347000
H	6.51851800	-4.42251800	-3.63589900
H	5.60973200	-5.56458600	-2.60964500
H	5.83843300	-3.88170000	-2.09056500
C	4.43213600	-2.68359900	-4.16744400
H	5.33487100	-2.50992600	-4.77356500
H	4.46053200	-1.99421700	-3.31059700
H	3.55280300	-2.42221000	-4.77337800
C	4.24044900	-5.03924600	-4.93737600
H	5.13752100	-4.92502200	-5.56502500
H	3.37222900	-4.77227700	-5.55890100
H	4.15600700	-6.10236200	-4.66328000
C	-0.32320100	-5.90993700	-2.74864500
C	-0.81685500	-5.38584500	-4.10560500
H	-1.70235000	-5.95206300	-4.43554500
H	-0.05131300	-5.48448700	-4.88926500
H	-1.09573500	-4.32493000	-4.03994100
C	0.10245300	-7.38010900	-2.89597300
H	-0.74772600	-7.99454700	-3.23375300
H	0.45787200	-7.78366100	-1.93521800
H	0.91480500	-7.49619300	-3.62915400
C	-1.48293300	-5.84368300	-1.75108800
H	-2.33591600	-6.42477400	-2.13421500
H	-1.83113600	-4.81239100	-1.59227200
H	-1.21053500	-6.27067300	-0.77407800
C	1.61341900	-5.54483500	4.12754600

C	0.64222500	-6.51140500	3.44401900
H	0.27395100	-7.24856100	4.17433700
H	1.12266800	-7.07184600	2.62754400
H	-0.23210600	-5.98381800	3.03174800
C	2.82243500	-6.34542100	4.63658500
H	2.50055200	-7.14273500	5.32660700
H	3.53384600	-5.70047600	5.17430400
H	3.36315700	-6.81184000	3.79862600
C	0.88501300	-4.91051400	5.32133200
H	0.55853200	-5.68930300	6.02931800
H	-0.00527100	-4.35624800	4.99032900
H	1.52758200	-4.20892800	5.87327800
C	6.13704300	1.08758900	5.25908900
C	7.10620500	0.09048600	5.91243200
H	7.55341100	0.52174500	6.82314900
H	7.92098600	-0.17284700	5.22038100
H	6.59769700	-0.84232700	6.19876000
C	5.01281900	1.43181300	6.24824400
H	5.42669300	1.87500300	7.16883700
H	4.43433900	0.54108200	6.53547800
H	4.30929100	2.15313600	5.80477000
C	6.90752700	2.37267100	4.94779000
H	7.31382400	2.79930100	5.87804500
H	6.25951200	3.13458300	4.48726800
H	7.75490400	2.18825800	4.26978500
C	5.51285200	1.14687300	0.27012500
C	5.39149600	2.54077300	0.18002300
H	4.97669900	3.07426000	1.03310400
C	5.74611000	3.23623400	-0.97638100
C	6.29919200	2.49998900	-2.02884300
H	6.60271500	3.02700900	-2.93651800
C	6.48619700	1.11336400	-1.96286400
C	6.04847200	0.44283600	-0.81571300
H	6.14306900	-0.63908700	-0.72413900
C	5.52286200	4.74437100	-1.13198700
C	4.92601600	5.37221700	0.12990700
H	4.77788400	6.45225600	-0.02460200
H	5.58860800	5.24827000	1.00015300
H	3.94821800	4.93341200	0.38137500
C	6.85970800	5.43675200	-1.43449400
H	6.71461100	6.52263200	-1.55376700
H	7.31756300	5.05774900	-2.36027300
H	7.57735200	5.27421000	-0.61566100
C	4.54428100	4.98375100	-2.29328500
H	4.36627500	6.06191200	-2.43598500
H	3.57406600	4.50302500	-2.09032800
H	4.92648000	4.57753400	-3.24185100
C	7.16032100	0.39923000	-3.13915100
C	8.50733800	1.07157100	-3.44809700
H	9.00969600	0.55317800	-4.28062900
H	9.17262700	1.03707700	-2.57164300
H	8.38940500	2.12589200	-3.73848600
C	6.24736300	0.50023300	-4.37113900
H	6.69113900	-0.02760600	-5.23097400
H	6.08786200	1.54840500	-4.66683000
H	5.26076900	0.05762100	-4.17080400
C	7.43647900	-1.07241600	-2.82880800
H	7.91999200	-1.55548400	-3.69211300
H	6.51669900	-1.63054300	-2.61456200
H	8.10794800	-1.17972600	-1.96327500
N	0.00418200	0.37118500	-1.79021800
H	3.14591700	0.26940400	-2.20458600
H	3.04739300	1.17315500	-0.66718300
Ca	-1.44045400	1.29593600	-0.14107100
Si	1.06783200	1.67462200	-2.26484500
Si	-0.48880100	-0.72763400	-3.07888500
C	2.83005300	1.22425100	-1.74721300
N	-3.79403300	1.14902800	-0.61540000
C	0.49182000	3.27193400	-1.42293600
C	1.16821400	2.15316800	-4.08224100
C	-1.36406000	0.08448800	-4.53948500
C	-1.61650300	-2.05668100	-2.38899500
C	1.03150700	-1.60873700	-3.76916800
H	3.55107600	1.97383600	-2.10769300
C	-3.66327700	2.15501400	-1.55284700
C	-4.33747600	0.07846100	-1.31275200
H	1.23488300	4.07119300	-1.57481200

H	-0.43999300	3.60412200	-1.91099200
H	0.33121000	3.24506300	-0.33168100
H	1.87550100	2.99488500	-4.16810700
H	1.53475100	1.34299600	-4.72902200
H	0.19185700	2.48601400	-4.46329400
H	-2.06521100	-0.64128300	-4.98144100
H	-1.94703500	0.96394000	-4.23403300
H	-0.65652300	0.39271800	-5.32256000
H	-2.07811400	-2.60525900	-3.22242800
H	-1.05625200	-2.78134200	-1.78154700
H	-2.44773700	-1.65176700	-1.79469700
H	0.74459400	-2.33547800	-4.54622800
H	1.74457800	-0.90228900	-4.22167200
H	1.56958400	-2.17866100	-2.99457300
C	-3.17231300	3.47899200	-1.38743700
C	-4.03606800	1.72312200	-2.86443100
C	-4.46581600	0.36402700	-2.70559900
C	-4.73520100	-1.20213100	-0.85910300
C	-3.03207200	4.25780200	-2.55269100
C	-2.91771900	4.13735100	-0.07891000
C	-3.89594700	2.54112100	-3.97934000
C	-4.86300100	-0.59858800	-3.63270300
C	-5.12756000	-2.13896600	-1.82561100
C	-4.83116200	-1.62710500	0.55744400
H	-2.70089900	5.28640500	-2.41832500
C	-3.36346100	3.82735600	-3.84430100
C	-3.70478300	3.86263100	1.04770200
C	-1.96619200	5.17557200	0.00875300
H	-4.19314200	2.16101100	-4.96044900
H	-4.91395800	-0.32899900	-4.69122900
C	-5.17439800	-1.88949400	-3.20787200
H	-5.43619500	-3.11602300	-1.45336900
C	-4.31236800	-2.87099000	0.94181100
C	-5.56687500	-0.87955000	1.48505600
C	-3.18806800	4.71655400	-5.07984500
H	-4.42938500	3.04852500	0.97849700
C	-3.62189800	4.65685000	2.20383500
C	-1.82831400	5.95616700	1.15036800
H	-1.33293200	5.37108100	-0.85361600
C	-5.57310700	-2.96347900	-4.22633000
H	-3.74368200	-3.43540200	0.20223700
C	-4.51505600	-3.38458800	2.22513300
C	-5.81652500	-1.37141100	2.76940800
H	-5.96637400	0.08151200	1.16137900
C	-2.57338900	6.07477200	-4.73428300
C	-4.55690300	4.95677000	-5.73461500
C	-2.25803700	4.01203400	-6.08002200
C	-2.68422000	5.68925300	2.23133600
C	-4.57502700	4.39026600	3.37363700
C	-0.79115200	7.07936700	1.25366600
C	-6.88124100	-2.54840300	-4.91646900
C	-4.46377700	-3.10809100	-5.28008200
C	-5.78001500	-4.33186500	-3.57220600
C	-5.27141600	-2.61484800	3.11588800
C	-3.96786000	-4.74647100	2.67071400
C	-6.66914400	-0.61951600	3.79687000
H	-2.44607000	6.67104100	-5.65093000
H	-3.21341900	6.65316400	-4.05031500
H	-1.58110700	5.96635000	-4.26866700
H	-4.45352100	5.59064600	-6.63039400
H	-5.03002800	4.01333000	-6.04542300
H	-5.24235000	5.45901500	-5.03465600
H	-2.13221800	4.62167700	-6.98946900
H	-1.26211900	3.84765000	-5.64001600
H	-2.65125200	3.03111300	-6.38584100
H	-2.60062100	6.30730900	3.12501600
C	-6.02401600	4.42991400	2.86291100
C	-4.27253400	3.00787400	3.96334300
C	-4.43377100	5.42919700	4.48795000
C	0.18538600	6.77023600	2.39883800
C	-1.51173500	8.40682000	1.53430200
C	0.02234600	7.23353400	-0.03383500
H	-7.18839600	-3.30291400	-5.65933100
H	-7.69275600	-2.43914800	-4.18059900
H	-6.77369100	-1.58585500	-5.43900300
H	-4.74424200	-3.85822100	-6.03733300
H	-4.26913600	-2.16141700	-5.80584900

H	-3.52022700	-3.43382500	-4.81517900
H	-6.03266000	-5.07892900	-4.34070300
H	-4.86929200	-4.67613100	-3.05679400
H	-6.60332900	-4.31878900	-2.84187500
H	-5.45463800	-3.00432000	4.12010900
C	-3.20182500	-5.45894900	1.55298900
C	-5.13903300	-5.64604000	3.09513600
C	-3.01528200	-4.55045100	3.85964200
C	-7.86165500	-1.49740700	4.20725300
C	-5.81070500	-0.31027600	5.03327300
C	-7.21757700	0.69303700	3.23542700
H	-6.72669200	4.23817400	3.68945500
H	-6.26025100	5.41491500	2.43153900
H	-6.21009800	3.67278700	2.08785700
H	-4.99139500	2.76048500	4.75986200
H	-4.32883900	2.21861100	3.20064300
H	-3.26183100	2.98140600	4.39843800
H	-5.14878600	5.20576200	5.29448900
H	-3.42622800	5.42167600	4.93157100
H	-4.64582300	6.44776600	4.12774000
H	0.91293200	7.58962800	2.51383100
H	-0.33550000	6.64658100	3.36014900
H	0.74481600	5.84377600	2.19811900
H	-0.78437400	9.23134300	1.60540000
H	-2.22315500	8.64491800	0.72853000
H	-2.07371600	8.37670500	2.47958400
H	0.75464100	8.04679100	0.08423700
H	0.58304500	6.31688000	-0.27454200
H	-0.61507100	7.48397200	-0.89588600
H	-2.83436100	-6.43198000	1.91404700
H	-3.83711100	-5.64802000	0.67435300
H	-2.32623800	-4.88256300	1.21848500
H	-4.76937800	-6.63377800	3.41461500
H	-5.70485500	-5.21406200	3.93375500
H	-5.84026800	-5.79506400	2.25964200
H	-2.62523600	-5.51928300	4.21029900
H	-2.15514900	-3.92621500	3.57393700
H	-3.51407400	-4.06103500	4.70930500
H	-8.48969300	-0.97108000	4.94413300
H	-8.48732300	-1.74060900	3.33463400
H	-7.53795500	-2.44546600	4.66200400
H	-6.39349800	0.25650000	5.77749100
H	-5.45331900	-1.23014000	5.52015500
H	-4.92817300	0.28596400	4.75971800
H	-7.81654200	1.20813800	4.00241300
H	-6.41331400	1.37654900	2.93200200
H	-7.86738400	0.52188000	2.36381700

4.2.3 [(^{dtbp}Cbz)Ca(C_6H_6)H]$_2$

0 1

Ca	-1.33435700	-1.07551100	-0.03353600
H	-0.82256000	1.01408200	-0.05830000
N	-2.77868600	-1.31756800	1.81488100
C	-3.37567400	-0.22852200	2.40892200
C	-4.30992600	0.67257400	1.85712400
C	-4.69197700	1.77113100	2.63213300
H	-5.42183300	2.45071000	2.18954500
C	-4.21575900	2.01544500	3.93631200
C	-3.32224200	1.09301500	4.48472900
H	-2.93543300	1.22956600	5.49880800
C	-2.90650500	-0.01252700	3.74022900
C	-1.96216000	-1.07033900	3.98605200
C	-1.10662400	-1.37964200	5.04301600
H	-1.14349600	-0.77570900	5.95397500
C	-0.17749200	-2.42014400	4.92157000
C	-0.16963900	-3.16015100	3.72323300
H	0.52032900	-3.99742700	3.61155100
C	-1.03607800	-2.90877000	2.65144800
C	-1.93931200	-1.82881300	2.77459400
C	-4.94319600	0.47065600	0.53045400
C	-5.71488800	-0.67516000	0.29058400
H	-5.74486200	-1.43683900	1.06943500
C	-6.45952400	-0.81216000	-0.88397300
C	-6.36661400	0.20825000	-1.84233000
H	-6.94009500	0.11123900	-2.76665100
C	-5.57889200	1.34966100	-1.65804300

C	-4.87816100	1.46634200	-0.45123500
H	-4.26623800	2.34343000	-0.24286100
C	-7.36332700	-2.02050000	-1.15561300
C	-7.47197000	-2.93890800	0.06343100
H	-6.49706900	-3.34711000	0.36362100
H	-8.12966100	-3.79107700	-0.16772500
H	-7.89901300	-2.40939900	0.92867900
C	-6.78924400	-2.82182800	-2.33454300
H	-6.71538800	-2.20749200	-3.24485000
H	-7.42880300	-3.68967500	-2.56331600
H	-5.78154000	-3.19976000	-2.10395900
C	-8.77821300	-1.53743200	-1.51027100
H	-8.79165100	-0.92217500	-2.42193600
H	-9.20276600	-0.93560600	-0.69207900
H	-9.44315200	-2.39868500	-1.68334700
C	-5.56396000	2.45008400	-2.72672700
C	-5.32205000	1.85523300	-4.12203000
H	-5.30751200	2.65555400	-4.87868900
H	-6.10854800	1.14380300	-4.41270900
H	-4.35855300	1.32696400	-4.17659500
C	-6.93125800	3.15300000	-2.70883800
H	-6.96468100	3.95772500	-3.46128900
H	-7.13030900	3.59627300	-1.72097100
H	-7.74635900	2.44686100	-2.92873200
C	-4.47885100	3.49508600	-2.45509700
H	-3.47317800	3.04613100	-2.41420100
H	-4.64917600	4.02635400	-1.50779000
H	-4.47251400	4.24881800	-3.25727600
C	-4.65956900	3.22899000	4.76336000
C	-5.62183000	4.13757300	3.99437400
H	-5.16336700	4.53502700	3.07557800
H	-5.90579300	4.99708900	4.62132700
H	-6.54671500	3.61087700	3.71407400
C	-3.42733300	4.06052800	5.15410800
H	-2.90147000	4.42549800	4.25877500
H	-2.71031100	3.47253800	5.74635500
H	-3.72228100	4.93427800	5.75827000
C	-5.37265400	2.74567900	6.03571900
H	-5.69823100	3.60150800	6.64987200
H	-4.71505900	2.11852300	6.65602500
H	-6.26068700	2.14673900	5.78120700
C	0.79993900	-2.70702700	6.06798000
C	1.62704800	-1.44404500	6.35730600
H	2.19873400	-1.13708500	5.46769700
H	2.34110400	-1.62605200	7.17710700
H	0.99109600	-0.59552800	6.65014800
C	0.01194300	-3.10257800	7.32565800
H	-0.68058400	-2.30620000	7.63701100
H	0.69512500	-3.30213000	8.16755800
H	-0.58417700	-4.01008100	7.14345300
C	1.77235400	-3.84009100	5.73103500
H	2.38196900	-3.60497800	4.84480700
H	1.24771700	-4.78968100	5.54469600
H	2.46214000	-4.00246500	6.57386700
C	-0.99144100	-3.77875800	1.45012600
C	0.23017400	-4.07723700	0.83750800
H	1.12495600	-3.57004500	1.20300600
C	0.31864300	-4.99842800	-0.21576100
C	-0.85734100	-5.62401200	-0.63324700
H	-0.80525500	-6.36723800	-1.42808400
C	-2.10949500	-5.33462000	-0.06361300
C	-2.16286300	-4.38604300	0.95985700
H	-3.10575100	-4.12238400	1.43855700
C	1.68756200	-5.29998400	-0.83030900
C	2.34782200	-3.99088200	-1.28267600
H	3.37888100	-4.17325900	-1.61957000
H	2.37943100	-3.23361700	-0.48747000
H	1.80815300	-3.53338300	-2.12490500
C	2.55847200	-5.97528000	0.24121300
H	3.56306500	-6.19079300	-0.15763300
H	2.10876100	-6.92424200	0.57221300
H	2.67746100	-5.33514300	1.12687100
C	1.59391600	-6.23482500	-2.03755900
H	0.96301400	-5.81099700	-2.83494000
H	1.18994300	-7.22273600	-1.76742300
H	2.59677800	-6.39387000	-2.46268500
C	-3.34918300	-6.13091500	-0.48922900

C	-3.29366600	-7.49390400	0.22087400
H	-4.17221800	-8.10557700	-0.04187200
H	-3.27706800	-7.36511500	1.31383200
H	-2.38906500	-8.05249200	-0.06489900
C	-3.38269200	-6.36467100	-2.00635900
H	-3.39751500	-5.41834300	-2.56852500
H	-4.28947000	-6.92677900	-2.27836000
H	-2.52246300	-6.95069100	-2.36055700
C	-4.63985100	-5.41349700	-0.08840900
H	-4.66919600	-4.38925900	-0.48888200
H	-4.75930100	-5.34779400	1.00275400
H	-5.51495300	-5.95383700	-0.48040600
C	-2.47049000	-2.53819400	-2.25844400
H	-3.01930400	-3.44181700	-1.99197500
C	-1.10678300	-2.61898500	-2.56059500
H	-0.60507000	-3.58750000	-2.52411000
C	-0.38501700	-1.45861600	-2.86743200
H	0.68563200	-1.50512700	-3.08255500
C	-1.03622000	-0.22082200	-2.87330800
H	-0.48016000	0.68999000	-3.09088700
C	-2.39995300	-0.14425100	-2.57763100
H	-2.89498100	0.82612300	-2.54655400
C	-3.12359700	-1.29872100	-2.27011700
H	-4.18242900	-1.22372500	-2.01674400
H	0.82258800	-1.01408500	0.05842300
Ca	1.33438400	1.07552900	0.03361800
N	2.77862800	1.31752700	-1.81486200
C	3.12347400	1.29875500	2.27029200
C	3.37561000	0.22843800	-2.40883300
C	2.39972300	0.14434500	2.57778800
H	2.89467000	-0.82607500	2.54675600
C	1.93922800	1.82868700	-2.77459800
C	2.47045500	2.53827600	2.25854700
H	4.18232300	1.22368100	2.01700400
C	4.30991800	-0.67257500	-1.85699800
C	2.90638100	0.01230400	-3.74009700
C	1.03597800	0.22102900	2.87339200
C	1.96203700	1.07010500	-3.98599100
C	1.03604800	2.90869600	-2.65156400
H	3.01935200	3.44184800	1.99207300
C	1.10673500	2.61917500	2.56061600
C	4.69197800	-1.77118200	-2.63192900
C	4.94321500	-0.47056800	-0.53035000
C	3.32212400	-1.09328900	-4.48451800
C	0.38486800	1.45887200	2.86746200
H	0.47983900	-0.68973900	3.09094600
C	1.10649700	1.37933300	-5.04297500
C	0.16961100	3.16001600	-3.72336400
C	0.99143900	3.77876300	-1.45030000
H	0.60509300	3.58772400	2.52407100
H	5.42186100	-2.45070900	-2.18930400
C	4.21569600	-2.01563800	-3.93605600
C	5.71489700	0.67526100	-0.29053700
C	4.87821400	-1.46622600	0.45137600
H	2.93525200	-1.22996100	-5.49855600
H	-0.68578700	1.50546600	3.08253700
H	1.14332500	0.77529300	-5.95386400
C	0.17740400	2.41988400	-4.92162100
H	-0.52030300	3.99734700	-3.61175500
C	-0.23016300	4.07734800	-0.83772000
C	2.16289800	4.38598100	-0.96002500
C	4.65950200	-3.22925700	-4.76299400
H	5.74484700	1.43691600	-1.06941400
C	6.45956300	0.81230800	0.88399700
C	5.57900700	-1.34951300	1.65814600
H	4.26629300	-2.34332700	0.24304100
C	-0.80008600	2.70666500	-6.06800600
H	-1.12497800	3.57021200	-1.20321700
C	-0.31859000	4.99860900	0.21549000
C	2.10957100	5.33463300	0.06337600
H	3.10577500	4.12222400	-1.43869300
C	5.62161300	-4.13786100	-3.99384800
C	3.42725900	-4.06074200	-5.15382800
C	5.37275800	-2.74604900	-6.03529900
C	6.36670500	-0.20807800	1.84237900
C	7.36334700	2.02067300	1.15558800
C	5.56417600	-2.44991400	2.72684700

C	-1.62722300	1.44366200	-6.35716500
C	-0.01216300	3.10209400	-7.32576600
C	-1.77248000	3.83976200	-5.73110200
C	0.85742500	5.62414000	0.63296800
C	-1.68750000	5.30027600	0.82998700
C	3.34929300	6.13089700	0.48895000
H	5.16302300	-4.53521700	-3.07507000
H	5.90557600	-4.99744000	-4.62071400
H	6.54651100	-3.61122200	-3.71348600
H	2.90127500	-4.42563100	-4.25853300
H	2.71033400	-3.47275000	-5.74619100
H	3.72222400	-4.93453900	-5.75791200
H	5.69836300	-3.60192500	-6.64937400
H	4.71526100	-2.11888700	-6.65570400
H	6.26079200	-2.14714100	-5.78071600
H	6.94020400	-0.11102400	2.76668400
C	7.47188500	2.93909300	-0.06345800
C	6.78931300	2.82195900	2.33456900
C	8.77827700	1.53765600	1.51014700
C	5.32277500	-1.85498800	4.12220200
C	6.93134600	-3.15307400	2.70858200
C	4.47880600	-3.49472300	2.45553600
H	-2.19886900	1.13679500	-5.46749900
H	-2.34131900	1.62559900	-7.17694700
H	-0.99129700	0.59510800	-6.64995300
H	0.68034700	2.30568600	-7.63708000
H	-0.69539300	3.30156000	-8.16764800
H	0.58396500	4.00961600	-7.14368700
H	-2.38206500	3.60471900	-4.84483100
H	-1.24782700	4.78936200	-5.54485400
H	-2.46229800	4.00207600	-6.57391700
H	0.80537200	6.36741800	1.42775800
C	-2.34782000	3.99123200	1.28242500
C	-2.55834800	5.97553300	-0.24161100
C	-1.59384300	6.23519500	2.03717700
C	3.29390800	7.49379400	-0.22134200
C	3.38273200	6.36486800	2.00604700
C	4.63993900	5.41334300	0.08829900
H	6.49696100	3.34729600	-0.36356800
H	8.12959500	3.79125900	0.16764900
H	7.89885700	2.40958800	-0.92874400
H	6.71554900	2.20760000	3.24486700
H	7.42884700	3.68983100	2.56331400
H	5.78157300	3.19984400	2.10406400
H	8.79181100	0.92241000	2.42181600
H	9.20279100	0.93584100	0.69192700
H	9.44319600	2.39893700	1.68316500
H	5.30833000	-2.65528100	4.87889200
H	6.10947500	-1.14367800	4.41262700
H	4.35937900	-1.32655900	4.17702800
H	6.96483300	-3.95780400	3.46102400
H	7.13004600	-3.59638300	1.72066000
H	7.74663200	-2.44707900	2.92825000
H	3.47320000	-3.04559200	2.41494500
H	4.64875900	-4.02600700	1.50817100
H	4.47258400	-4.24846600	3.25770400
H	-3.37888200	4.17368300	1.61927500
H	-2.37943200	3.23392100	0.48726600
H	-1.80818700	3.53376300	2.12469300
H	-3.56293100	6.19116600	0.15719800
H	-2.10855800	6.92442600	-0.57269900
H	-2.67737600	5.33531400	-1.12720700
H	-0.96296300	5.81139900	2.83459400
H	-1.18984000	7.22307800	1.76698500
H	-2.59670700	6.39429700	2.46227800
H	4.17248200	8.10544700	0.04137600
H	3.27737000	7.36485500	-1.31428400
H	2.38932400	8.05247600	0.06429800
H	3.39741300	5.41862100	2.56835200
H	4.28955300	6.92691800	2.27802500
H	2.52254400	6.95103200	2.36010300
H	4.66917100	4.38913700	0.48886400
H	4.75946800	5.34752900	-1.00284900
H	5.51505300	5.95364900	0.48031300

4.2.4 [(^{dtbp}Cbz)Yb(C_6H_6)H]$_2$

0 1

Yb	-1.91406000	-0.17014000	-0.56453700
H	-0.14953200	1.25020200	0.01178800
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C	-3.18990100	0.71085200	2.51020800
C	-3.20399500	2.09343000	2.22975900
C	-2.88476700	2.97454800	3.26809700
H	-2.89759600	4.03937400	3.03053500
C	-2.58935200	2.55694900	4.58272400
C	-2.61884200	1.18557100	4.85352300
H	-2.39515000	0.81688000	5.85902100
C	-2.90405000	0.27026800	3.83859700
C	-2.88716700	-1.16733700	3.75836000
C	-2.58464500	-2.18143600	4.66863500
H	-2.38199900	-1.91982000	5.71175400
C	-2.52054100	-3.51363200	4.24975500
C	-2.79124700	-3.79149100	2.89473900
H	-2.76693300	-4.82337600	2.54077500
C	-3.11343700	-2.80975800	1.95303800
C	-3.15432700	-1.46607100	2.38691900
C	-3.56138300	2.63696300	0.89529900
C	-4.82837700	2.38409600	0.33488200
H	-5.49351600	1.71007800	0.87498800
C	-5.24672000	3.03766200	-0.82479800
C	-4.33808000	3.90311500	-1.46291600
H	-4.66133100	4.41969700	-2.36744100
C	-3.06432200	4.15764900	-0.95638900
C	-2.69399400	3.50731000	0.23187400
H	-1.71740200	3.69012200	0.68190300
C	-6.67833400	2.93521700	-1.36629500
C	-7.55334000	2.01532200	-0.51305800
H	-7.15554800	0.99190100	-0.47200100
H	-8.56631000	1.96081000	-0.94077000
H	-7.64672300	2.38672400	0.51850000
C	-6.66542700	2.40632700	-2.80736300
H	-6.04373400	3.02830100	-3.46905600
H	-7.68548800	2.39394900	-3.22331500
H	-6.28049700	1.37720500	-2.84232000
C	-7.30978400	4.33782200	-1.34886400
H	-6.76865400	5.04185800	-1.99823000
H	-7.31002200	4.75343000	-0.32951000
H	-8.35275400	4.29196600	-1.70146200
C	-2.11095800	5.18281700	-1.57920700
C	-2.62225600	5.72885000	-2.91357700
H	-1.88308700	6.42626700	-3.33696600
H	-3.56890200	6.27901500	-2.80100100
H	-2.77631900	4.92700900	-3.65334500
C	-1.97442700	6.35647500	-0.59365600
H	-1.31435500	7.13487500	-1.00950500
H	-1.54581500	6.03065100	0.36504100
H	-2.95580300	6.81043500	-0.38664800
C	-0.73119000	4.55618200	-1.81332400
H	-0.73968700	3.84593600	-2.65089300
H	-0.36783100	4.00277600	-0.93772400
H	0.00692900	5.33466200	-2.05936800
C	-2.23803600	3.54652000	5.70143500
C	-2.33377900	5.00269100	5.24022500
H	-1.63339000	5.21759900	4.41932900
H	-2.08220500	5.67621300	6.07428100
H	-3.34955000	5.25654500	4.90029700
C	-0.79818200	3.28761300	6.17374800
H	-0.08164500	3.44407900	5.35216100
H	-0.66755600	2.25614900	6.53443300
H	-0.52745900	3.96994900	6.99634600
C	-3.20348200	3.35704800	6.88130600
H	-2.96674200	4.06306100	7.69418400
H	-3.14760800	2.34015000	7.29713400
H	-4.24374000	3.53151800	6.56581200
C	-2.15558400	-4.60895600	5.25962600
C	-0.77668400	-4.30160200	5.86689200
H	-0.00556700	-4.26283900	5.08201600
H	-0.48695500	-5.07821900	6.59374000
H	-0.76903900	-3.33484200	6.39238300
C	-3.20781000	-4.64751400	6.37828700
H	-3.27432600	-3.68389300	6.90512300

H	-2.95955200	-5.42193300	7.12282100
H	-4.20443300	-4.87140000	5.96764800
C	-2.09158500	-5.99651300	4.61634200
H	-1.33512400	-6.04394100	3.81717400
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H	-1.82010900	-6.74826500	5.37372500
C	-3.36579800	-3.18292900	0.54108500
C	-2.46405500	-3.99910600	-0.15376000
H	-1.55752800	-4.31249000	0.36472600
C	-2.69491800	-4.39911500	-1.47482100
C	-3.88405000	-3.98464400	-2.08587600
H	-4.09378500	-4.30897900	-3.10317500
C	-4.82043900	-3.17802200	-1.42330000
C	-4.52759900	-2.75784900	-0.12068500
H	-5.22359600	-2.12414200	0.43275300
C	-1.66590200	-5.28819900	-2.18135800
C	-0.28925400	-4.61277300	-2.13733600
H	0.47595900	-5.25816900	-2.59621800
H	0.01961500	-4.40422200	-1.10552800
H	-0.28239400	-3.64917600	-2.66627100
C	-1.58955800	-6.63470500	-1.44334500
H	-0.85551500	-7.29865100	-1.92786900
H	-2.56696800	-7.14153200	-1.44584700
H	-1.28143000	-6.50337700	-0.39514400
C	-2.02901300	-5.55438400	-3.64340200
H	-2.11056100	-4.62109700	-4.22263200
H	-2.97980100	-6.10065600	-3.74040900
H	-1.24591200	-6.16628500	-4.11656300
C	-6.17114700	-2.80808300	-2.04619000
C	-7.28646600	-3.45935200	-1.21176800
H	-8.27514900	-3.22277200	-1.63728800
H	-7.27205000	-3.10416900	-0.17081100
H	-7.17263100	-4.55416000	-1.19364700
C	-6.30671400	-3.29499900	-3.49069200
H	-5.52891100	-2.87478200	-4.14807600
H	-7.28205000	-2.98684500	-3.89722000
H	-6.25207200	-4.39192800	-3.56021500
C	-6.34917000	-1.28618200	-2.02619500
H	-5.59168500	-0.79386400	-2.65289600
H	-6.25134500	-0.87767200	-1.01058700
H	-7.34146400	-1.00073800	-2.40930900
C	-2.90996900	-0.77089000	-3.74450300
H	-3.73123700	-1.48705700	-3.80774300
C	-1.58854500	-1.21202500	-3.86144600
H	-1.38100900	-2.27023200	-4.02921600
C	-0.53025100	-0.30431500	-3.75331300
H	0.50276400	-0.65160100	-3.83067600
C	-0.79240400	1.05330400	-3.53663600
H	0.04268800	1.75308000	-3.44720300
C	-2.11557100	1.49778900	-3.43189500
H	-2.33484500	2.55168000	-3.25224600
C	-3.17405500	0.58806500	-3.53165000
H	-4.20137800	0.94690100	-3.44036500
H	-0.09317100	-1.59307900	-0.32180200
Yb	1.63925700	-0.20041500	0.34914700
N	3.36605900	0.21069000	-1.60947300
C	2.94113400	-0.70689600	3.74013200
C	3.30773400	-0.85371600	-2.47480300
C	1.68371400	-1.08873200	4.21397800
H	1.54930200	-2.06310000	4.68928600
C	3.10508800	1.31450700	-2.38249700
C	3.10404400	0.55011800	3.14829900
H	3.79328900	-1.38394800	3.82500000
C	3.41866400	-2.22574300	-2.16730300
C	3.00042900	-0.45840000	-3.81136800
C	0.58731100	-0.23591700	4.06950800
C	2.86574900	0.97420200	-3.75099100
C	2.99441500	2.66352300	-1.97394000
H	4.08040900	0.86360100	2.77304000
C	2.01040200	1.41859900	3.02556700
C	3.17809200	-3.14963900	-3.18603200
C	3.73211700	-2.68444400	-0.78973300
C	2.79169800	-1.41402400	-4.80889200
C	0.74520000	1.01798900	3.47169600
H	-0.40159900	-0.55321300	4.40309400
C	2.50255600	1.94762800	-4.68292600
C	2.61498100	3.60199600	-2.94087500

C	3.30947000	3.11439000	-0.59695700
H	2.15541900	2.39854800	2.56325300
H	3.25246200	-4.20569300	-2.92201800
C	2.86167200	-2.77813100	-4.50999800
C	4.97794600	-2.40595300	-0.19962600
C	2.79733100	-3.43548700	-0.07261600
H	2.53920300	-1.08256700	-5.82041300
H	-0.12371200	1.67173600	3.35448900
H	2.31678200	1.65163000	-5.71941300
C	2.35993200	3.28177300	-4.29026600
H	2.55321200	4.64218100	-2.61869500
C	2.49893700	4.05084300	0.05158000
C	4.48614700	2.68988400	0.04593500
C	2.55652000	-3.81286700	-5.60073900
H	5.69025100	-1.81592400	-0.77596900
C	5.30651000	-2.91050500	1.05847900
C	3.07304900	-3.92213100	1.21768200
H	1.83810000	-3.64229200	-0.54960600
C	1.94162000	4.33710900	-5.32304000
H	1.57474800	4.35386100	-0.43830700
C	2.84708400	4.60326100	1.29093800
C	4.88881300	3.24557600	1.26287300
H	5.09819800	1.94652600	-0.46424100
C	2.79986900	-5.24766600	-5.12627300
C	1.07830600	-3.68647400	-6.00596000
C	3.44629000	-3.56169400	-6.82709700
C	4.33019600	-3.64911300	1.75391600
C	6.69620500	-2.74004900	1.68314500
C	2.01099700	-4.74799400	1.94784100
C	0.52547500	4.01735700	-5.82882800
C	2.92085800	4.31936800	-6.50677800
C	1.93215700	5.75236700	-4.74032900
C	4.05273400	4.19916800	1.86824800
C	1.90450600	5.61445900	1.95292900
C	6.26151100	2.93123600	1.87008300
H	2.14709700	-5.51698600	-4.28198300
H	2.58739700	-5.95339500	-5.94441300
H	3.84409300	-5.40100800	-4.81350300
H	0.42280000	-3.88652100	-5.14383000
H	0.84585400	-2.67699100	-6.37804400
H	0.82453300	-4.40709800	-6.80106500
H	3.23455100	-4.30011700	-7.61763900
H	3.28346900	-2.56176600	-7.25541600
H	4.51116300	-3.64046200	-6.55904700
H	4.57950500	-4.03667100	2.74223600
C	7.64738600	-1.96831800	0.76643900
C	6.57839400	-1.99285200	3.02009400
C	7.30257400	-4.13074400	1.93308300
C	2.44752500	-5.13760800	3.36102900
C	1.74923000	-6.03579500	1.14987800
C	0.71390700	-3.93477500	2.04267100
H	-0.20332000	4.06018900	-5.00426200
H	0.21051400	4.74263300	-6.59720300
H	0.46958300	3.01130800	-6.27144900
H	2.93713200	3.34196000	-7.01107100
H	2.63760500	5.07637300	-7.25641500
H	3.94548400	4.53685000	-6.16789600
H	1.21325100	5.84970300	-3.91305400
H	2.92531700	6.04649000	-4.36777400
H	1.63920200	6.47476000	-5.51805900
H	4.36097700	4.63861200	2.81567400
C	0.56320200	4.92939100	2.25507000
C	1.67154600	6.79086500	0.99200700
C	2.46775100	6.16458900	3.26429500
C	7.22516900	4.05257000	1.44626100
C	6.21250100	2.87750100	3.40367500
C	6.80290600	1.59439600	1.35926800
H	7.27607400	-0.95962200	0.53957600
H	8.62873300	-1.85973700	1.25330700
H	7.80511500	-2.49579900	-0.18642300
H	5.95373200	-2.54265000	3.74073100
H	7.57166000	-1.86195100	3.47823600
H	6.13969500	-0.99380100	2.87973300
H	6.69531000	-4.72676200	2.63050300
H	7.38512700	-4.69591900	0.99201300
H	8.31143000	-4.03577500	2.36584000
H	1.64675300	-5.70939600	3.85401900

H	3.34878200	-5.76986100	3.35491700
H	2.65337700	-4.25287300	3.98369700
H	0.97853600	-6.64546500	1.64903900
H	1.39661900	-5.81936200	0.13113000
H	2.66517300	-6.64107100	1.06594500
H	0.85087400	-3.03163400	2.65462700
H	0.35507600	-3.59775700	1.06017900
H	-0.09052300	-4.52176500	2.50930000
H	-0.17046300	5.66127100	2.62892300
H	0.14039100	4.45245400	1.36025300
H	0.67414600	4.14831700	3.02222200
H	1.00522000	7.53781600	1.45266700
H	2.62229400	7.28562800	0.74038500
H	1.20253800	6.46476800	0.05230700
H	2.63129000	5.36677900	4.00532800
H	3.42098000	6.69349900	3.11024700
H	1.75644500	6.88056100	3.70391500
H	8.23644300	3.86909700	1.84506100
H	7.29236400	4.11658800	0.34949600
H	6.88116100	5.02970200	1.81889700
H	5.50321400	2.11868400	3.76722400
H	7.20799500	2.62551000	3.80105900
H	5.92485800	3.84164300	3.84699600
H	6.08198100	0.77980900	1.52583600
H	7.02702300	1.61986300	0.28298000
H	7.73609100	1.33380100	1.88152900

4.2.5 [(^{dtbp}Cbz)Ca(C_6H_6)H]$_2$ – C_6H_6 removed

0 1

Ca	-1.33435700	-1.07551100	-0.03353600
H	-0.82256000	1.01408200	-0.05830000
N	-2.77868600	-1.31756800	1.81488100
C	-3.37567400	-0.22852200	2.40892200
C	-4.30992600	0.67257400	1.85712400
C	-4.69197700	1.77113100	2.63213300
H	-5.42183300	2.45071000	2.18954500
C	-4.21575900	2.01544500	3.93631200
C	-3.32224200	1.09301500	4.48472900
H	-2.93543300	1.22956600	5.49880800
C	-2.90650500	-0.01252700	3.74022900
C	-1.96216000	-1.07033900	3.98605200
C	-1.10662400	-1.37964200	5.04301600
H	-1.14349600	-0.77570900	5.95397500
C	-0.17749200	-2.42014400	4.92157000
C	-0.16963900	-3.16015100	3.72323300
H	0.52032900	-3.99742700	3.61155100
C	-1.03607800	-2.90877000	2.65144800
C	-1.93931200	-1.82881300	2.77459400
C	-4.94319600	0.47065600	0.53045400
C	-5.71488800	-0.67516000	0.29058400
H	-5.74486200	-1.43683900	1.06943500
C	-6.45952400	-0.81216000	-0.88397300
C	-6.36661400	0.20825000	-1.84233000
H	-6.94009500	0.11123900	-2.76665100
C	-5.57889200	1.34966100	-1.65804300
C	-4.87816100	1.46634200	-0.45123500
H	-4.26623800	2.34343000	-0.24286100
C	-7.36332700	-2.02050000	-1.15561300
C	-7.47197000	-2.93890800	0.06343100
H	-6.49706900	-3.34711000	0.36362100
H	-8.12966100	-3.79107700	-0.16772500
H	-7.89901300	-2.40939900	0.92867900
C	-6.78924400	-2.82182800	-2.33454300
H	-6.71538800	-2.20749200	-3.24485000
H	-7.42880300	-3.68967500	-2.56331600
H	-5.78154000	-3.19976000	-2.10395900
C	-8.77821300	-1.53743200	-1.51027100
H	-8.79165100	-0.92217500	-2.42193600
H	-9.20276600	-0.93560600	-0.69207900
H	-9.44315200	-2.39868500	-1.68334700
C	-5.56396000	2.45008400	-2.72672700
C	-5.32205000	1.85523300	-4.12203000
H	-5.30751200	2.65555400	-4.87868900
H	-6.10854800	1.14380300	-4.41270900

H	-4.35855300	1.32696400	-4.17659500
C	-6.93125800	3.15300000	-2.70883800
H	-6.96468100	3.95772500	-3.46128900
H	-7.13030900	3.59627300	-1.72097100
H	-7.74635900	2.44686100	-2.92873200
C	-4.47885100	3.49508600	-2.45509700
H	-3.47317800	3.04613100	-2.41420100
H	-4.64917600	4.02635400	-1.50779000
H	-4.47251400	4.24881800	-3.25727600
C	-4.65956900	3.22899000	4.76336000
C	-5.62183000	4.13757300	3.99437400
H	-5.16336700	4.53502700	3.07557800
H	-5.90579300	4.99708900	4.62132700
H	-6.54671500	3.61087700	3.71407400
C	-3.42733300	4.06052800	5.15410800
H	-2.90147000	4.42549800	4.25877500
H	-2.71031100	3.47253800	5.74635500
H	-3.72228100	4.93427800	5.75827000
C	-5.37265400	2.74567900	6.03571900
H	-5.69823100	3.60150800	6.64987200
H	-4.71505900	2.11852300	6.65602500
H	-6.26068700	2.14673900	5.78120700
C	0.79993900	-2.70702700	6.06798000
C	1.62704800	-1.44404500	6.35730600
H	2.19873400	-1.13708500	5.46769700
H	2.34110400	-1.62605200	7.17710700
H	0.99109600	-0.59552800	6.65014800
C	0.01194300	-3.10257800	7.32565800
H	-0.68058400	-2.30620000	7.63701100
H	0.69512500	-3.30213000	8.16755800
H	-0.58417700	-4.01008100	7.14345300
C	1.77235400	-3.84009100	5.73103500
H	2.38196900	-3.60497800	4.84480700
H	1.24771700	-4.78968100	5.54469600
H	2.46214000	-4.00246500	6.57386700
C	-0.99144100	-3.77875800	1.45012600
C	0.23017400	-4.07723700	0.83750800
H	1.12495600	-3.57004500	1.20300600
C	0.31864300	-4.99842800	-0.21576100
C	-0.85734100	-5.62401200	-0.63324700
H	-0.80525500	-6.36723800	-1.42808400
C	-2.10949500	-5.33462000	-0.06361300
C	-2.16286300	-4.38604300	0.95985700
H	-3.10575100	-4.12238400	1.43855700
C	1.68756200	-5.29998400	-0.83030900
C	2.34782200	-3.99088200	-1.28267600
H	3.37888100	-4.17325900	-1.61957000
H	2.37943100	-3.23361700	-0.48747000
H	1.80815300	-3.53338300	-2.12490500
C	2.55847200	-5.97528000	0.24121300
H	3.56306500	-6.19079300	-0.15763300
H	2.10876100	-6.92424200	0.57221300
H	2.67746100	-5.33514300	1.12687100
C	1.59391600	-6.23482500	-2.03755900
H	0.96301400	-5.81099700	-2.83494000
H	1.18994300	-7.22273600	-1.76742300
H	2.59677800	-6.39387000	-2.46268500
C	-3.34918300	-6.13091500	-0.48922900
C	-3.29366600	-7.49390400	0.22087400
H	-4.17221800	-8.10557700	-0.04187200
H	-3.27706800	-7.36511500	1.31383200
H	-2.38906500	-8.05249200	-0.06489900
C	-3.38269200	-6.36467100	-2.00635900
H	-3.39751500	-5.41834300	-2.56852500
H	-4.28947000	-6.92677900	-2.27836000
H	-2.52246300	-6.95069100	-2.36055700
C	-4.63985100	-5.41349700	-0.08840900
H	-4.66919600	-4.38925900	-0.48888200
H	-4.75930100	-5.34779400	1.00275400
H	-5.51495300	-5.95383700	-0.48040600
H	0.82258800	-1.01408500	0.05842300
Ca	1.33438400	1.07552900	0.03361800
N	2.77862800	1.31752700	-1.81486200
C	3.37561000	0.22843800	-2.40883300
C	1.93922800	1.82868700	-2.77459800
C	4.30991800	-0.67257500	-1.85699800
C	2.90638100	0.01230400	-3.74009700

C	1.96203700	1.07010500	-3.98599100
C	1.03604800	2.90869600	-2.65156400
C	4.69197800	-1.77118200	-2.63192900
C	4.94321500	-0.47056800	-0.53035000
C	3.32212400	-1.09328900	-4.48451800
C	1.10649700	1.37933300	-5.04297500
C	0.16961100	3.16001600	-3.72336400
C	0.99143900	3.77876300	-1.45030000
H	5.42186100	-2.45070900	-2.18930400
C	4.21569600	-2.01563800	-3.93605600
C	5.71489700	0.67526100	-0.29053700
C	4.87821400	-1.46622600	0.45137600
H	2.93525200	-1.22996100	-5.49855600
H	1.14332500	0.77529300	-5.95386400
C	0.17740400	2.41988400	-4.92162100
H	-0.52030300	3.99734700	-3.61175500
C	-0.23016300	4.07734800	-0.83772000
C	2.16289800	4.38598100	-0.96002500
C	4.65950200	-3.22925700	-4.76299400
H	5.74484700	1.43691600	-1.06941400
C	6.45956300	0.81230800	0.88399700
C	5.57900700	-1.34951300	1.65814600
H	4.26629300	-2.34332700	0.24304100
C	-0.80008600	2.70666500	-6.06800600
H	-1.12497800	3.57021200	-1.20321700
C	-0.31859000	4.99860900	0.21549000
C	2.10957100	5.33463300	0.06337600
H	3.10577500	4.12222400	-1.43869300
C	5.62161300	-4.13786100	-3.99384800
C	3.42725900	-4.06074200	-5.15382800
C	5.37275800	-2.74604900	-6.03529900
C	6.36670500	-0.20807800	1.84237900
C	7.36334700	2.02067300	1.15558800
C	5.56417600	-2.44991400	2.72684700
C	-1.62722300	1.44366200	-6.35716500
C	-0.01216300	3.10209400	-7.32576600
C	-1.77248000	3.83976200	-5.73110200
C	0.85742500	5.62414000	0.63296800
C	-1.68750000	5.30027600	0.82998700
C	3.34929300	6.13089700	0.48895000
H	5.16302300	-4.53521700	-3.07507000
H	5.90557600	-4.99744000	-4.62071400
H	6.54651100	-3.61122200	-3.71348600
H	2.90127500	-4.42563100	-4.25853300
H	2.71033400	-3.47275000	-5.74619100
H	3.72222400	-4.93453900	-5.75791200
H	5.69836300	-3.60192500	-6.64937400
H	4.71526100	-2.11888700	-6.65570400
H	6.26079200	-2.14714100	-5.78071600
H	6.94020400	-0.11102400	2.76668400
C	7.47188500	2.93909300	-0.06345800
C	6.78931300	2.82195900	2.33456900
C	8.77827700	1.53765600	1.51014700
C	5.32277500	-1.85498800	4.12220200
C	6.93134600	-3.15307400	2.70858200
C	4.47880600	-3.49472300	2.45553600
H	-2.19886900	1.13679500	-5.46749900
H	-2.34131900	1.62559900	-7.17694700
H	-0.99129700	0.59510800	-6.64995300
H	0.68034700	2.30568600	-7.63708000
H	-0.69539300	3.30156000	-8.16764800
H	0.58396500	4.00961600	-7.14368700
H	-2.38206500	3.60471900	-4.84483100
H	-1.24782700	4.78936200	-5.54485400
H	-2.46229800	4.00207600	-6.57391700
H	0.80537200	6.36741800	1.42775800
C	-2.34782000	3.99123200	1.28242500
C	-2.55834800	5.97553300	-0.24161100
C	-1.59384300	6.23519500	2.03717700
C	3.29390800	7.49379400	-0.22134200
C	3.38273200	6.36486800	2.00604700
C	4.63993900	5.41334300	0.08829900
H	6.49696100	3.34729600	-0.36356800
H	8.12959500	3.79125900	0.16764900
H	7.89885700	2.40958800	-0.92874400
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H	7.42884700	3.68983100	2.56331400

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 H                  7.74663200   -2.44707900    2.92825000
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 H                 -3.37888200    4.17368300    1.61927500
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 H                 -1.18984000    7.22307800    1.76698500
 H                 -2.59670700    6.39429700    2.46227800
 H                  4.17248200    8.10544700    0.04137600
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 H                  2.38932400    8.05247600    0.06429800
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 H                  4.66917100    4.38913700    0.48886400
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4.2.6 [(^{dtbp}Cbz)Ca(C_6H_6)H]$_2$ – flanking arene removed

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 C                 -4.69197700    1.77113100    2.63213300
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 C                 -4.21575900    2.01544500    3.93631200
 C                 -3.32224200    1.09301500    4.48472900
 H                 -2.93543300    1.22956600    5.49880800
 C                 -2.90650500   -0.01252700    3.74022900
 C                 -1.96216000   -1.07033900    3.98605200
 C                 -1.10662400   -1.37964200    5.04301600
 H                 -1.14349600   -0.77570900    5.95397500
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 C                 -1.93931200   -1.82881300    2.77459400
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C	3.12347400	1.29875500	2.27029200
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C	1.10649700	1.37933300	-5.04297500
C	0.16961100	3.16001600	-3.72336400
H	0.60509300	3.58772400	2.52407100
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C	4.21569600	-2.01563800	-3.93605600
H	2.93525200	-1.22996100	-5.49855600
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C	4.65950200	-3.22925700	-4.76299400
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C	5.62161300	-4.13786100	-3.99384800
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C	5.37275800	-2.74604900	-6.03529900
C	-1.62722300	1.44366200	-6.35716500
C	-0.01216300	3.10209400	-7.32576600
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H	2.90127500	-4.42563100	-4.25853300
H	2.71033400	-3.47275000	-5.74619100
H	3.72222400	-4.93453900	-5.75791200
H	5.69836300	-3.60192500	-6.64937400
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H	-2.19886900	1.13679500	-5.46749900
H	-2.34131900	1.62559900	-7.17694700
H	-0.99129700	0.59510800	-6.64995300
H	0.68034700	2.30568600	-7.63708000
H	-0.69539300	3.30156000	-8.16764800
H	0.58396500	4.00961600	-7.14368700
H	-2.38206500	3.60471900	-4.84483100
H	-1.24782700	4.78936200	-5.54485400
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H	1.00388226	3.53606593	-1.78538138
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H	-4.76657060	0.52697297	0.90047566

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