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SUPPORTING INFORMATION

Calcium Stilbene Complexes: Structures and Dual Reactivity

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1. Experimental Section

General Considerations

All experiments were carried out in dry glassware under N_2 using standard Schlenk-techniques and freshly dried and degassed solvents (all solvents were dried over a column except for THF which was dried over Na and redistilled). Following reagents were obtained commercially: iodine (99% ABCR), H_2 gas (5N, Alpha Gas). The following compounds were synthesized according to literature procedures: (tBuAm^{DIPP}CaH)$_2$ and (AdAm^{DIPP}CaH)$_2$.[1] NMR spectra were measured on Bruker Avance III HD 400 MHz or 600 MHz spectrometers. Elemental analysis was performed with a Hekatech Eurovector EA3000 analyzer. GC-MS analysis has been performed with a Thermo Scientic™ Trace™ 1310 gas chromatography system (carrier gas Helium) with detection by a Thermo Scientic™ ISQ™ LT Single Quadrupole mass spectrometer (EI-MS, 70 eV). Crystal structures have been measured on a SuperNova (Agilent) diffractometer with dual Cu and Mo microfocus sources and an Atlas S2 detector.

Synthesis of [tBuAm^{DIPP}Ca]$_2$(SD): In an NMR tube (tBuAm^{DIPP}CaH)$_2$ (50.0 mg; 54.3 μmol) was suspended in benzene (0.60 mL) and diphenylacetylene (10.7 mg; 59.7 μmol, 1.1 eq) was added. The white suspension was heated up to 80°C in a heating block. After a few minutes the suspension turned into a thick dark brown solution which was kept overnight at 80 °C. A small amount of solids was removed by centrifugation. The mother liquor was cooled to 4 °C and the crystalline red-brown product was isolated by centrifugation, washed with 0.5 mL of cold (-30 °C) n-pentane and dried under high vacuum. Yield: 53.1 mg, 89 %. Melting point: 176°C. Elemental analysis: Calculated for $C_{72}H_{98}Ca_2N_4$: C 78.63, H 8.98, N 5.09; Found: C 79.92, H 8.80, 4.21. As the complex crystallized with two ordered molecules of benzene in the asymmetric unit, it is likely that some co-solvent is retained after drying. The values agree better with $C_{72}H_{98}Ca_2N_4 \cdot (C_6H_6)_2$: C 80.33, H 8.83, N 4.46. Crystals suitable for X-ray diffraction can be easily grown by using the following two approaches: 1) The mother liquor after synthesis was cooled to 4°C very slowly in an isolated Dewar vessel. After 2 days nice block-like crystals could be isolated. 2) The mother liquor after synthesis was layered with 0.6 mL of cold n-pentane and was left to stand at 20 °C for several days. Slow diffusion of pentane in the mother liquor, gave very large block-like single crystals. IR (pure, cm^{-1}): ν = 3054 (w), 2959 (s), 2903 (s), 2878 (s), 2847 (s), 2321 (w), 2113 (w), 1906 (w), 1581 (m), 1523 (m), 1479 (s), 1420 (s), 1350 (s), 1324 (m), 1306 (m), 1262 (s), 1224 (m), 1183 (m), 1165 (m), 1096 (m), 1063 (m), 1014 (w), 969 (m), 926 (m), 881 (w), 856 (w), 833 (w), 812 (w), 784 (m), 756 (m), 721 (s), 696 (s), 671 (s), 558 (w), 543 (w), 515 (m), 498 (m), 446 (w), 419 (w). The highly air-sensitive complex is poorly soluble in C_6D_6 and

partially decomposes into homoleptic and other species (Figure S1). Decomposition of the complex is also observed in THF-d_8.

The same procedure was used for a larger scale experiment: (tBuAm^{DIPP}CaH)$_2$ (200.0 mg; 217.0 μmol) was suspended in benzene (5.0 mL) and diphenylacetylene (42.5 mg; 238.7 μmol, 1.1 eq) was added. The white suspension was stirred vigorously at 80°C for 6 hours, but already after a few minutes the suspension turned into a dark brown solution. The solution was then cooled down to RT and small amounts of insoluble particles were removed by centrifugation. The mother liquor was concentrated to approximately 2 mL and layered with n-pentane (2.0 mL). Complete solvent mixing by diffusion was obtained after 2 days after which some needle shaped crystals were already visible. To improve the crystalline yield the sample was cooled to 4 °C very slowly and after 1 day no further crystals formation was observed. The crystals were separated from the mother liquor, washed with 1.0 mL of cold (-30 °C) n-pentane and dried under high vacuum. From the separated mother liquor no further crystals were obtained, even after further concentration. Crystalline yield: 182.4 mg, 76.4 %. The scale-up procedure has a lower yield than the small scale NMR experiment because the compound crystallizes better from an NMR tube.

Synthesis of [AdAm^{DIPP}Ca]$_2$(SD): In an NMR tube (AdAm^{DIPP}CaH)$_2$ (40.0 mg; 37.1 μmol) was suspended in benzene (0.60 mL) and diphenylacetylene (8.0 mg ; 44.55 μmol, 1.2 eq) was added. The white suspension was heated overnight up to 80°C in a heating block. . A small amount of solids was removed by centrifugation. The mother liquor was cooled to 4 °C and the crystalline red-brown product was isolated by centrifugation, washed with 0.8 mL of cold n-pentane (-30 °C) and dried under high vacuum. Yield: 42.0 mg, 90%. Elemental analysis: Calculated for $C_{84}H_{110}N_4Ca_2$: C 80.33, H 8.83, N 4.46; Found: C 80.56, H 8.91, N 4.12. Melting point: 234°C. Crystals suitable for X-ray diffraction could be obtained using the same procedures as mentioned for [tBuAm^{DIPP}Ca]$_2$(SD) but in the second procedure the mother liquor was layered with Et_2O instead of n-hexane. IR (pure, cm^{-1}): ν = 2959 (m), 2903 (m), 2877 (m), 2847 (m), 2107 (w), 1581 (m), 1522 (w), 1478(s), 1410 (s), 1350 (s), 1324 (s), 1306 (s), 1236 (s), 1184 (m), 1164 (m), 1097 (w), 1062 (w), 1014 (w), 968 (m), 926 (m), 881 (w), 856 (w), 833 (w), 785 (m), 757 (m), 727 (s), 695 (s), 670 (s), 544 (w), 515 (m), 492 (m), 449 (w), 419 (w). The highly air-sensitive complex is poorly soluble in C_6D_6 and partially decomposes into homoleptic species of which (AdAm^{DIPP})$_2$Ca (Figure S2). Decomposition of the complex is also observed in THF-d_8.

Reaction of [tBuAm^{DIPP}Ca]$_2$(SD) with I_2 to give [tBu^{DIPP}AmCaI·(THF)$_2$]$_2$ (3) and Ph(H)C=C(H)Ph: Crystals of [tBuAm^{DIPP}Ca]$_2$(SD) (40.0 mg; 36.4 μmol) were suspended in n-hexane (300 μl) in a NMR tube and cooled to -30°C. Separately, iodine (10.1 mg; 40.0 μmol) was dissolved in n-hexane/THF

(5:1; 250 μl n-hexane/ 50 μl THF) and given dropwise to the suspension carefully while keeping the temperature close to -30°C. Warming up the NMR tube to room temperature resulted in a color change of the dark-brown suspension to pale yellow and a fine white precipitate separated. The NMR tube was placed at -30°C overnight and the precipitate was separated from the mother liquor by centrifugation, washed with n-pentane (100 μl) and then dried under vacuum. Single crystals suitable for X-ray diffraction could be obtained by dissolving the white precipitate in THF (100 μl, 67 °C) and layering the solution with n-hexane (500 μl) at room temperature. Nice block-like crystals grew overnight. The crystal structure shows a dimeric complex of constitution: $[tBu^{DIPP}AmCaI\cdot(THF)_2]_2$ (Figures S10-S11). Yield: 21.1 mg; 40%. Elemental analysis: Calculated for $C_{74}H_{118}N_4O_4I_2Ca_2$: C 60.80 H 8.14; Found: C 61.05 H 8.22.

CAUTION: the reaction can be exothermic. High temperatures promote Schlenk equilibria to give $Ca(tBuAm^{DIPP})_2$ and CaI_2 and should be avoided.

^{1}H NMR (600 MHz, THF): δ= 0.90 (s, 9H, tBu), 1.16 (d, *J* = 6.9 Hz, 12H, iPt), 1.27 (d, *J* = 6.9 Hz, 12H, iPr), 1.68 (s, 8H, CH_2-THF), 3.53 (Hept, *J* = 6.9 Hz, 4H, iPr), 3.54 (s, 8H, O-CH_2-THF), 6.80 (t, *J* = 7.6 Hz, 2H, para-H DIPP), 6.94 (d, *J* = 7.6 Hz, 4H, meta-H DIPP).

^{13}C NMR (151 MHz, THF): δ= 23.4 (CH_3-tBu), 26.5 (CH_2-THF), 27.1 (iPr), 29.2 (iPr), 31.7 (iPr), 45.9 (*C*-tBu), 68.4 (O-CH_2-THF), 122.5 (Ar), 123.8 (Ar), 141.7 (Ar), 148.1 (Ar), 176.5 (N*C*N).

GC-MS measurement of the mother liquor that was separated from the product contained *cis*- and *trans*-stilbene in a 10/90 ratio. *Cis*-stilbene: R_t = 9.03 min, m/z: 180.14 $[C_{12}H_{14}]^+$, 165.12 $[C_{11}H_{11}]^+$, 152.11 $[C_{10}H_{10}]^+$, 91.08 $[C_7H_7]^+$. *Trans*-stilbene: R_t = 10.19 min, m/z: 180.14 $[C_{12}H_{14}]^+$, 165.12 $[C_{11}H_{11}]^+$, 152.11 $[C_{10}H_{10}]^+$, 91.08 $[C_7H_7]^+$.

Reaction of $[tBuAm^{DIPP}Ca]_2$(SD) with H_2 to give $(tBuAm^{DIPP}CaH)_2$ and $PhCH_2CH_2Ph$: Crystals of $[tBuAm^{DIPP}Ca]_2$(SD) (40.0 mg; 36.4 μmol) were charged in a high pressure NMR tube and partially dissolved in C_6D_6 (300 μl), then hydrogen (6 bars) was pumped into the tube and the reaction was monitored at regular time intervals. After 2 days at 80°C the reaction was complete (> 98%) and crystals of the rather insoluble $(tBuAm^{DIPP}CaH)_2$ grew inside the tube. The crystals were separated from the mother liquor and dried under vacuum. Yield: 12.0 mg; 36%. The ^{1}H NMR data fit to those reported for $(tBuAm^{DIPP}CaH)_2$.[1]

Catalytic reduction of diphenylacetylene by H_2: Crystals of the catalyst $[tBuAm^{DIPP}Ca]_2$(SD) (10.0 mg; 9.1 μmol; 10 mol%) were charged in a high pressure NMR tube and dissolved in C_6D_6 (300 μl).

Subsequently, diphenylacetylene (16.5 mg; 91.0 μmol) was added to the solution and the tube was pressurized with hydrogen (6 bars). The reaction was monitored by ^{1}H NMR at regular time intervals. At room temperature, no catalytic activity was observed. Consistent with the synthesis (tBuAm^{DIPP}CaH)$_2$ from [tBuAm^{DIPP}Ca]$_2$(SD) and H_2 (*vide supra*), conversion requires higher temperatures. At 80°C the dark solution gets clearer over time. 1H NMR monitoring shows that stilbene (mostly *trans*) and 1,2-diphenylethane are formed. Also signals for (tBuAm^{DIPP}CaH)$_2$ can be observed. During the catalytic reaction some homoleptic Ca(tBuAm^{DIPP})$_2$ is formed as well (colourless crystals of the (tBu^{DIPP}Am-CaH)$_2$ appeared after 10 hours). After 24 h the conversion is estimated to be 80 % and after 48 h the conversion is essentially complete (97%).

2. Selected NMR spectra

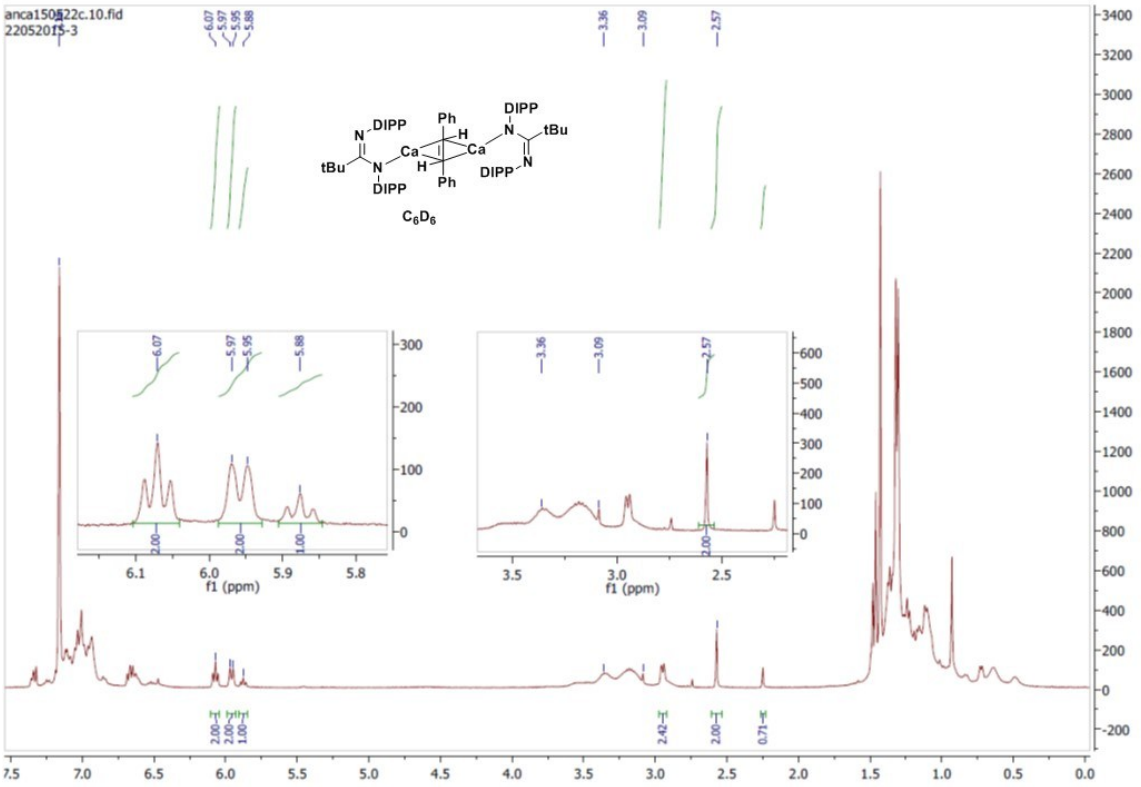
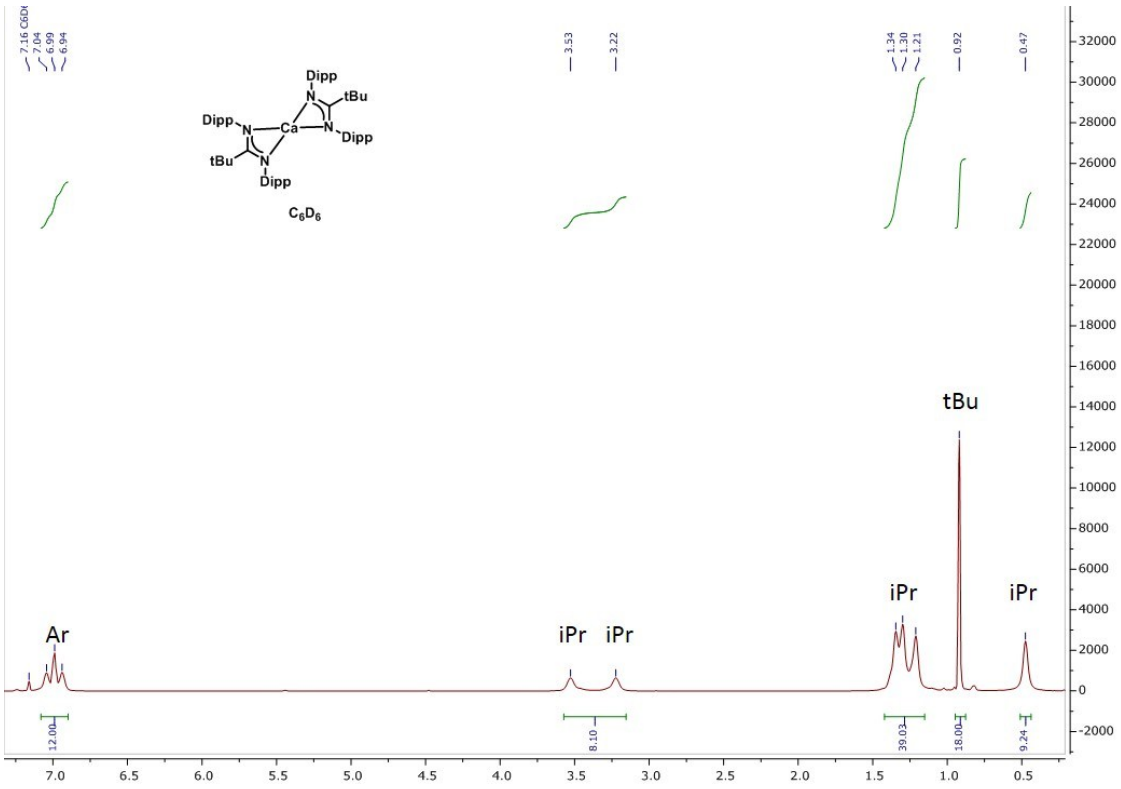


Figure S1. ^{1}H NMR spectrum of [*t*BuAm^{DIPP}Ca]$_2$(SD) in C_6D_6 (partial decomposition into homoleptic species). The doublet and triplets between 5.8-6.1 ppm and the singlet 2.57 ppm are tentatively assigned to SD. The homoleptic complex (*t*BuAm^{DIPP})$_2$Ca is identified by the broad signal at 0.5 ppm and the sharp singlet at 0.93 ppm (see also spectrum in Fig. S4 top) and the ^{1}H spectrum below for homoleptic [*t*BuAm^{DIPP}]$_2$Ca published by us in *Angew. Chem.* **2017**, *56*, 6906):



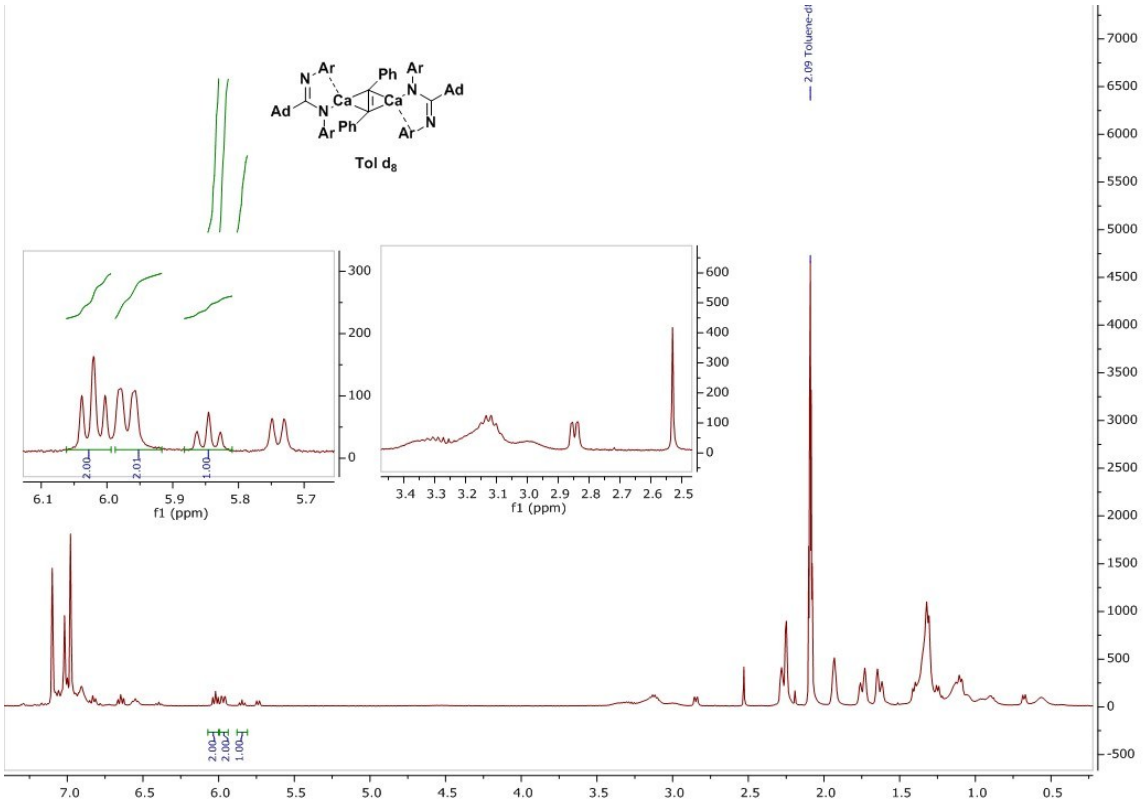


Figure S2. ^{1}H NMR spectrum of [AdAm^{DIPP}Ca]$_2$(SD) in toluene-d_8 (partial decomposition in homoleptic complexes). Typical for the homoleptic complex is the broad signal at high-field (0.6 ppm, iPr).

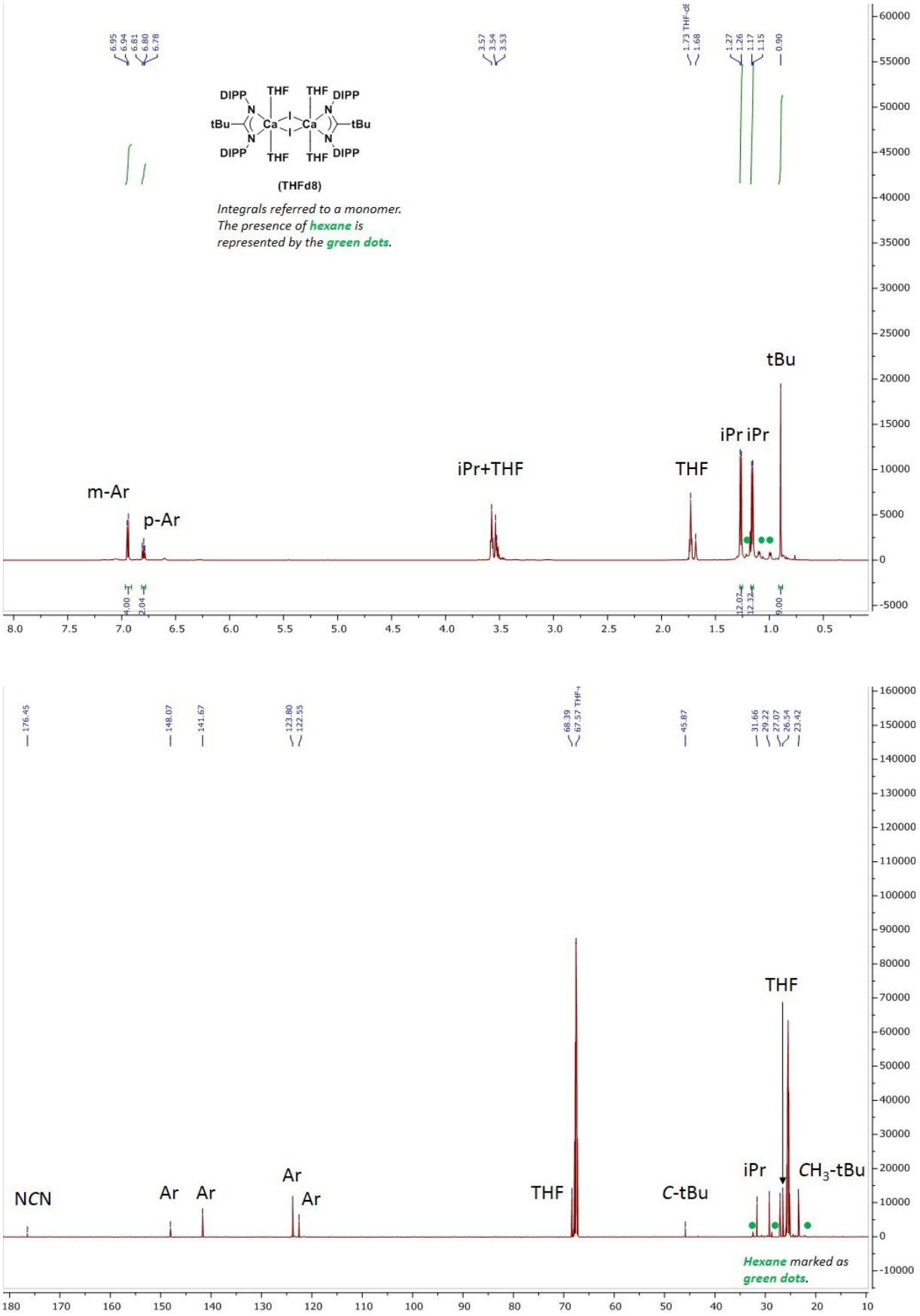


Figure S3. ^{1}H NMR (top) and ^{13}C{^{1}H} (bottom) NMR spectra of [tBu^{DIPP}AmCaI·(THF)$_2$]$_2$ in THF-d_8. The complex cocrystallizes with n-hexane, which is found as an impurity (labeled by green dots).

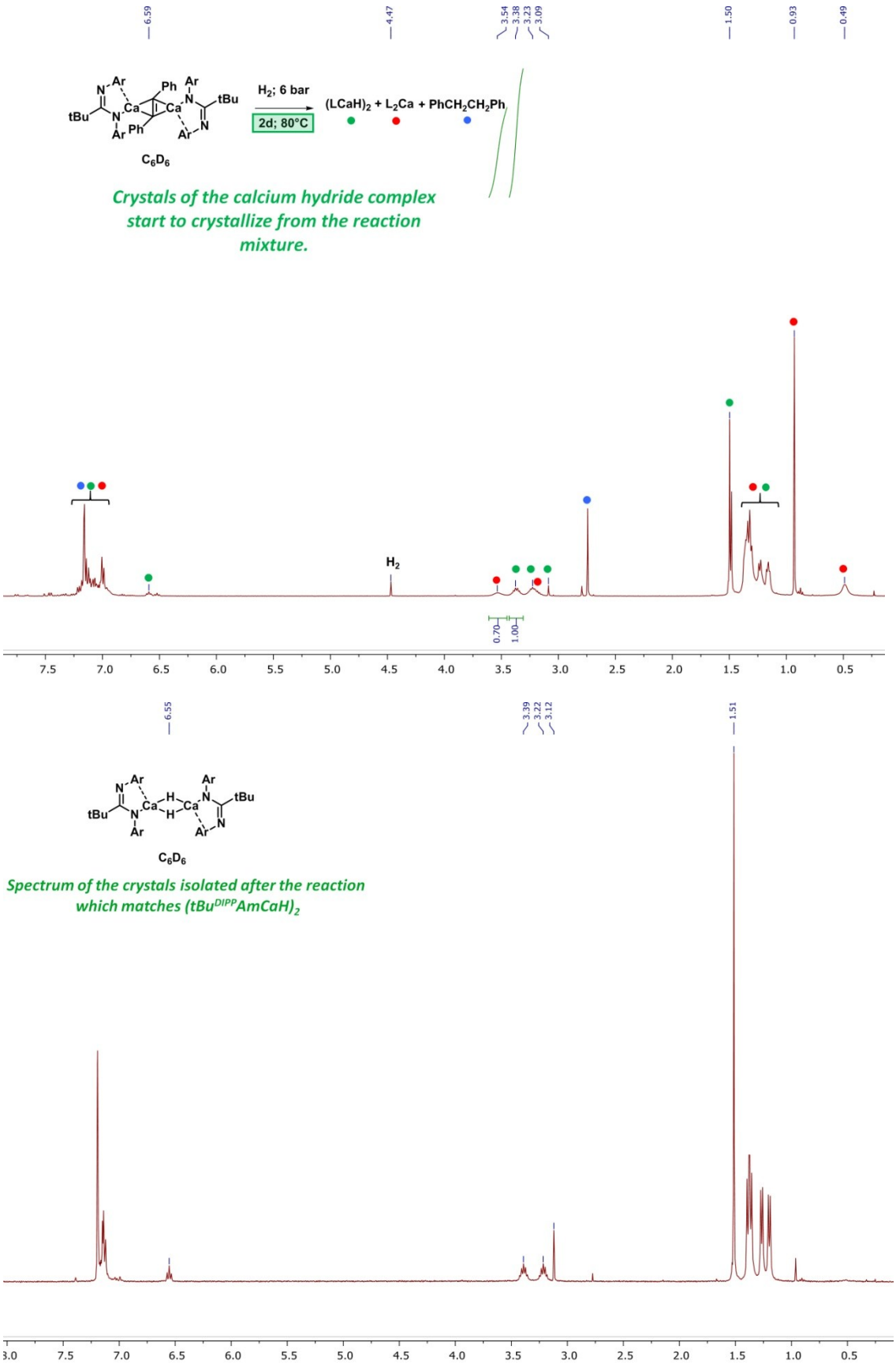


Figure S4. Top: ^{1}H NMR spectrum of the reaction of [*t*BuAm^{DIPP}Ca]$_2$(SD) with H_2 (6 bar, 80 °C, 48 h) in C_6D_6. Bottom: ^{1}H NMR spectrum of crystals of (*t*BuAm^{DIPP}CaH)$_2$ isolated from the reaction mixture (C_6D_6).

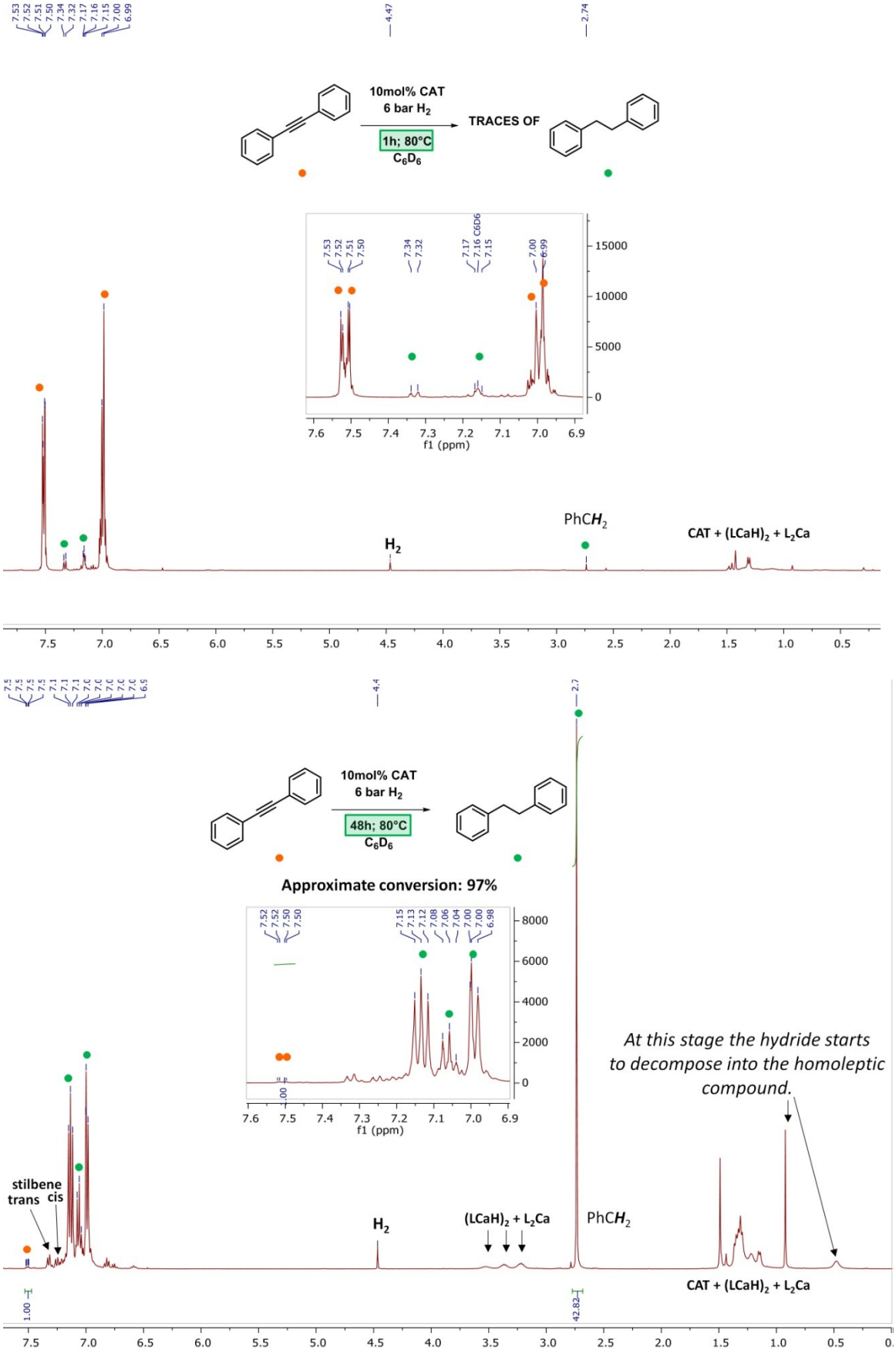


Figure S5. Catalytic conversion of diphenylacetylene into 1,2-diphenylethane: 10 mol% [*t*BuAm^{DIPP}Ca]$_2$(SD), 6 bar H_2, 80 °C, C_6D_6. Top: ^{1}H NMR spectrum after 1 hour. Bottom: ^{1}H NMR spectrum after 48 hours.

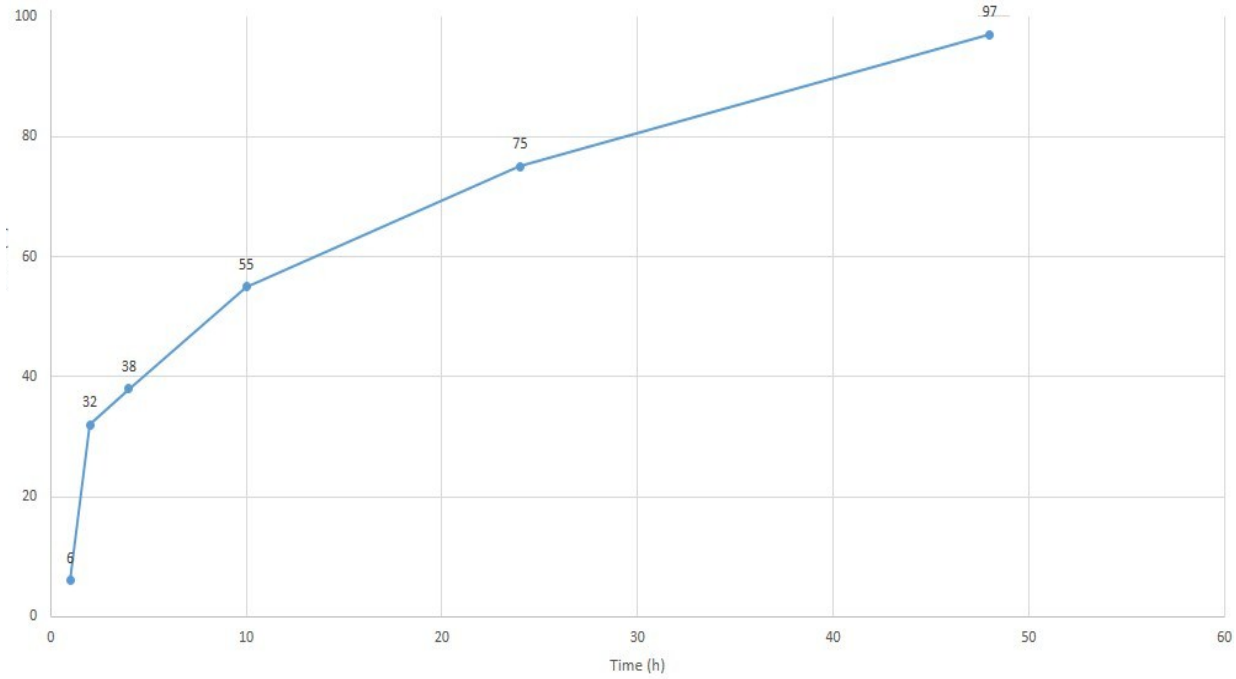


Figure S6. Conversion over time of the catalysis. The turn over number is 9.7. The initial turnover frequency (1/3 conversion) is 1.6 h^{-1}. The overall turnover frequency is 0.2 h^{-1}.

3. Selected IR spectra

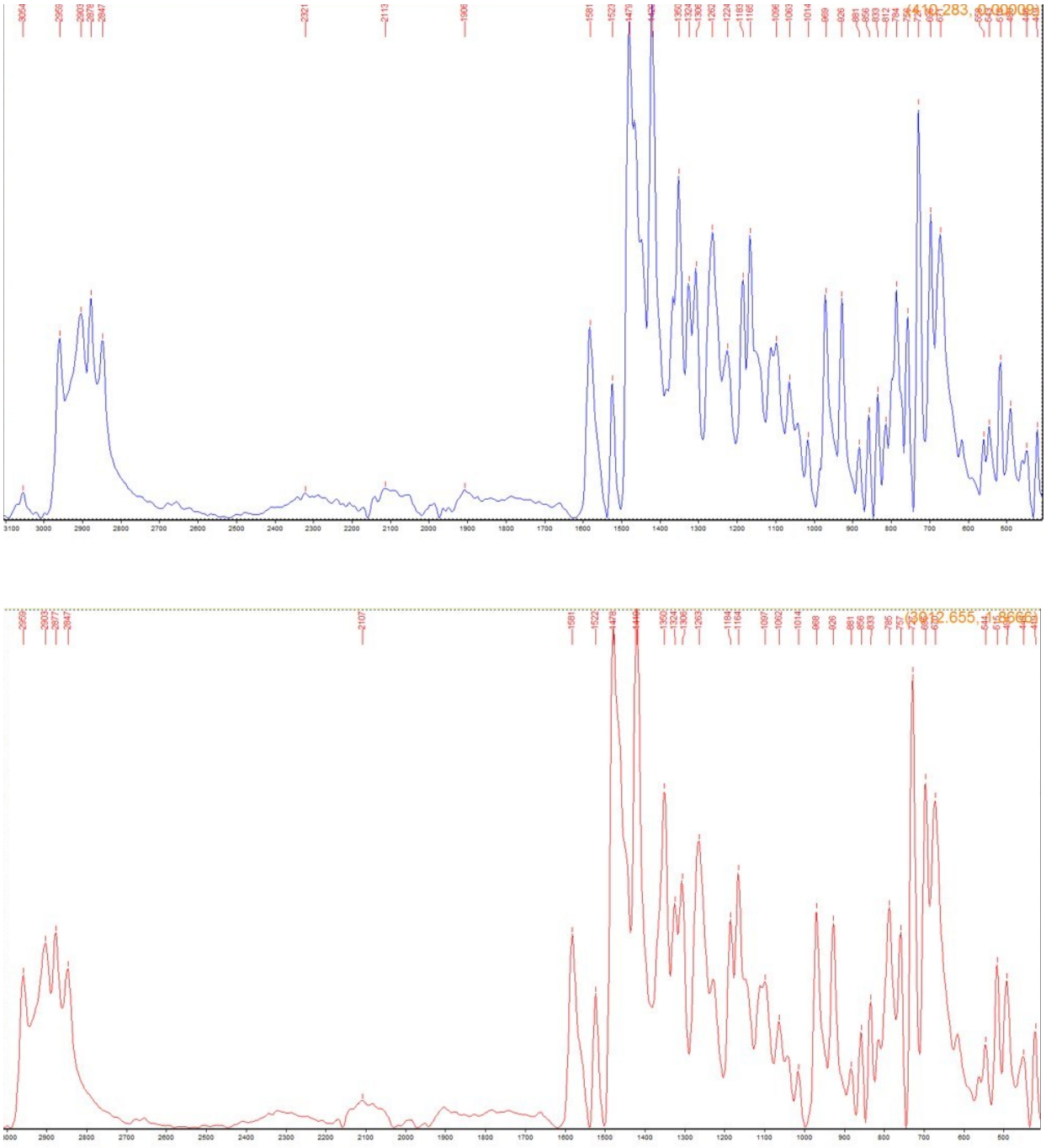


Figure S7. Infra-red spectrum of solid [*t*BuAm^{DIPP}Ca]$_2$(SD) (blue, top) and [AdAm^{DIPP}Ca]$_2$(SD) (red, bottom).

4. Crystal structures

General

Crystal structures have been measured on a SuperNova (Agilent) diffractometer with dual Cu and Mo microfocus sources and an Atlas S2 detector. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1560714 [*t*BuAm^{DIPP}Ca]$_2$(SD), 1560715 [AdAm^{DIPP}Ca]$_2$(SD) and 1560716 [*t*Bu^{DIPP}AmCaI·(THF)$_2$]$_2$. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)1223-336-033; E-mail: deposit@ccdc.cam.ac.uk).

Crystal structure of [*t*BuAm^{DIPP}Ca]$_2$(SD)

Using Olex2,[2] the structure was solved by Direct Methods (ShelXS)[3] and refined with ShelXL[4] using Least Squares minimization. All hydrogen atoms, except those from the benzylic carbons in the SD anion, have been placed on calculated positions and were refined isotropically in a riding model. The hydrogen atoms from the benzylic carbons could be localized and were refined isotropically. Two ordered benzene molecules cocrystallized in the asymmetric unit.

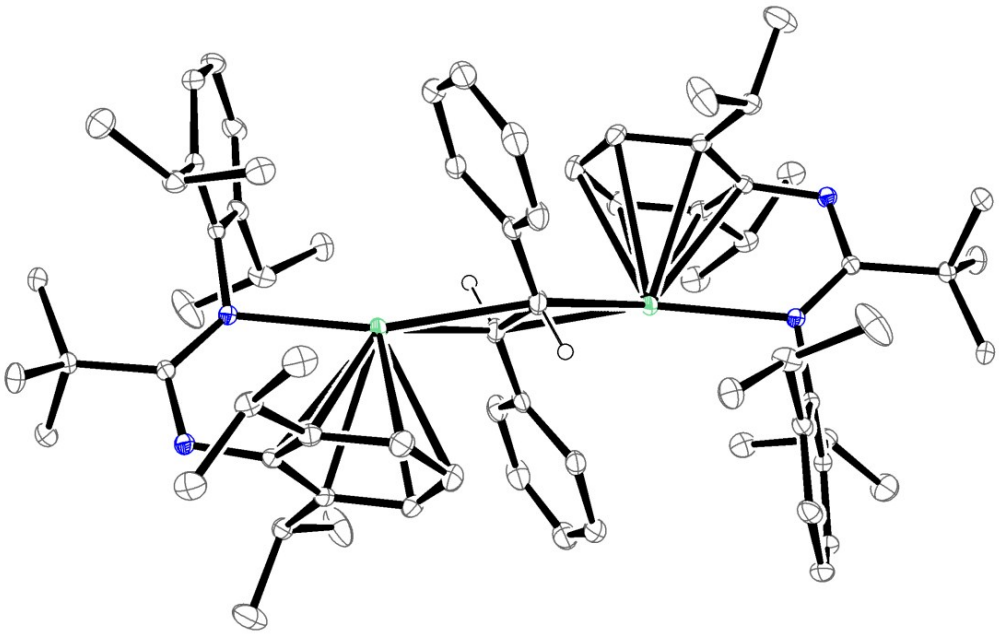


Figure S8. Crystal structure of [*t*BuAm^{DIPP}Ca]$_2$(SD); ORTEP plot (30% probability).

Table S1. Crystal data and structure refinement for *t*BuAm^{DIPP}Ca]$_2$(SD).

Identification code	hasj150420c
Empirical formula	$C_{96}H_{122}Ca_2N_4$
Formula weight	1412.13
Temperature/K	100.0(1)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.43516(13)
b/Å	10.43114(11)
c/Å	27.6902(3)
α/°	90
β/°	100.7627(10)
γ/°	90
Volume/Å^3	4096.11(8)
Z	2
ρ_{calc}g/cm^3	1.145
μ/mm^{-1}	1.563
F(000)	1532.0
Crystal color	Dark red
Crystal size/mm^3	0.361 × 0.26 × 0.18
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.468 to 147.13
Index ranges	-17 ≤ h ≤ 17, -12 ≤ k ≤ 10, -33 ≤ l ≤ 26
Reflections collected	14535
Independent reflections	7922 [R_{int} = 0.0291, R_{sigma} = 0.0366]
Data/restraints/parameters	7922/0/475
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0387, wR_2 = 0.1002
Final R indexes [all data]	R_1 = 0.0423, wR_2 = 0.1040
Largest diff. peak/hole / e Å^{-3}	0.28/-0.30

Crystal structure of [AdAm^{DIPP}Ca]$_2$(SD)

Using Olex2,[2] the structure was solved by Direct Methods (ShelXS)[3] and refined with ShelXL[4] using Least Squares minimization. All hydrogen atoms, except those from the benzylic carbons in the SD anion, have been placed on calculated positions and were refined isotropically in a riding model. The hydrogen atoms from the benzylic carbons could be localized and were refined isotropically. One ordered benzene molecule cocrystallized in the asymmetric unit.

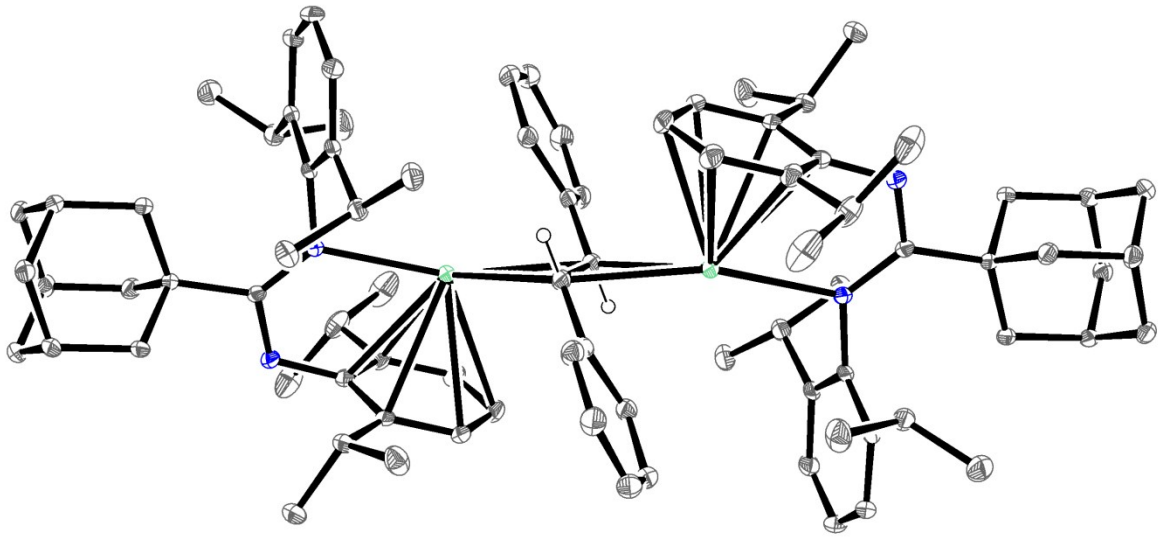


Figure S9. Crystal structure of [AdAm^{DIPP}Ca]$_2$(SD); ORTEP plot (30% probability).

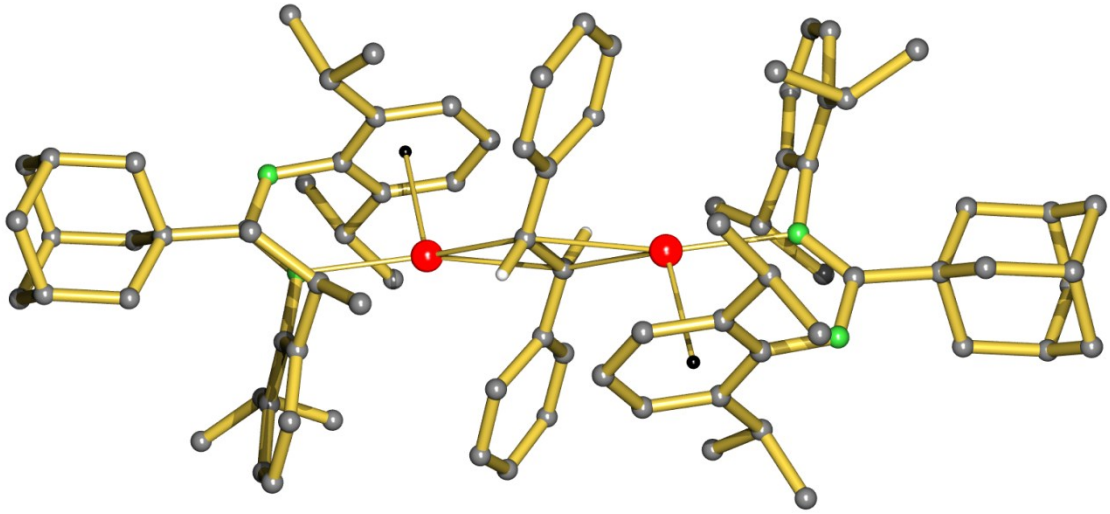


Figure S10. Crystal structure of [AdAm^{DIPP}Ca]$_2$(SD); Ball and stick plot.

Table S2. Crystal data and structure refinement for $[AdAm^{DIPP}Ca]_2$(SD)

Identification code	hasj170224b
Empirical formula	$C_{96}H_{122}Ca_2N_4$
Formula weight	1412.13
Temperature/K	100
Crystal system	triclinic
Space group	P-1
a/Å	10.3795(3)
b/Å	10.7062(4)
c/Å	20.4813(4)
α/°	101.777(2)
β/°	91.061(2)
γ/°	115.639(3)
Volume/Å^3	1993.93(10)
Z	1
ρ_{calc}g/cm^3	1.176
μ/mm^{-1}	1.602
F(000)	766.0
Crystal size/mm^3	0.174 × 0.091 × 0.054
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.886 to 136.234
Index ranges	-12 ≤ h ≤ 10, -12 ≤ k ≤ 12, -24 ≤ l ≤ 24
Reflections collected	18091
Independent reflections	7259 [R_{int} = 0.0356, R_{sigma} = 0.0374]
Data/restraints/parameters	7259/0/472
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0470, wR_2 = 0.1256
Final R indexes [all data]	R_1 = 0.0526, wR_2 = 0.1315
Largest diff. peak/hole / e Å^{-3}	0.43/-0.39

Crystal structure of $[t\text{Bu}^{DIPP}\text{AmCaI}\cdot(\text{THF})_2]_2$

Using Olex2,[2] the structure was solved by Direct Methods (ShelXS)[3] and refined with ShelXL[4] using Least Squares minimization. All hydrogen atoms have been placed on calculated positions and were refined isotropically in a riding model. The asymmetric unit contains cocrystallized *n*-hexane which is heavily disordered and was treated with the mask routine in OLEX (similar to SQUEEZE in PLATON). Per unit cell, a total of 1443 Å^3 voids (8.4%) have been masked with a total of 126 electrons.

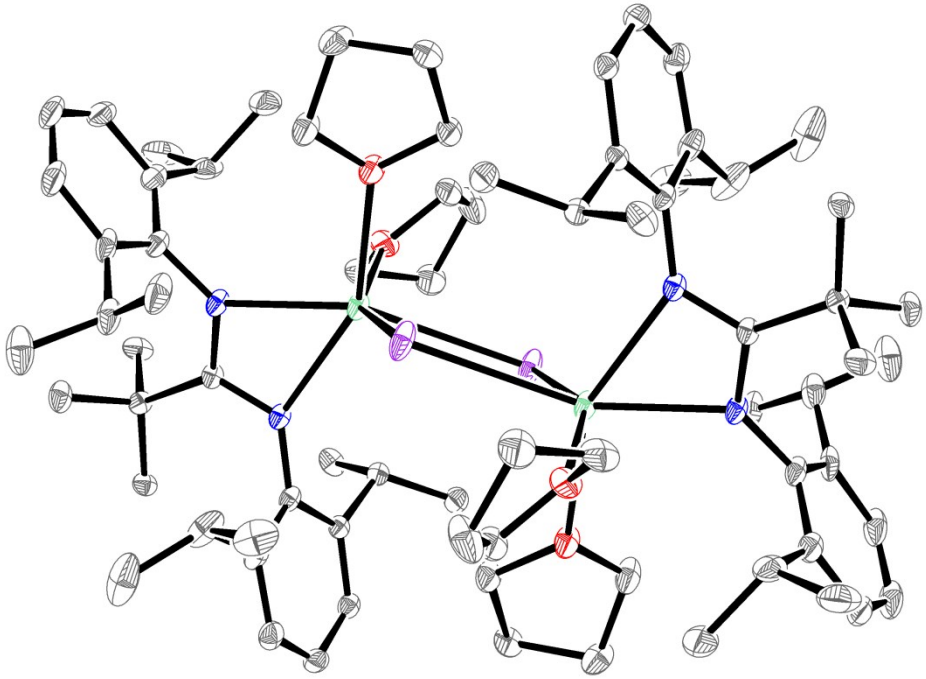


Figure S11. Crystal structure of [*t*Bu^{DIPP}AmCaI·(THF)$_2$]$_2$; ORTEP plot (30% probability).

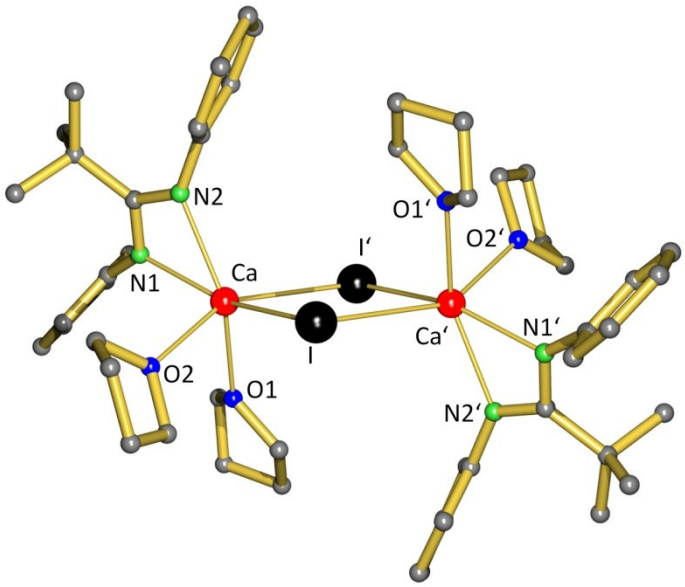


Figure S12. Crystal structure of [*t*Bu^{DIPP}AmCaI·(THF)$_2$]$_2$; Ball and stick plot.

Table S3. Crystal data and structure refinement for [*t*Bu^{DIPP}AmCaI·(THF)$_2$]$_2$.

Identification code	hasj170608b
Empirical formula	$C_{74}H_{118}Ca_2I_2N_4O_4$
Formula weight	1461.68
Temperature/K	100.01(10)
Crystal system	trigonal
Space group	R-3
a/Å	29.2848(9)
b/Å	29.2848(9)
c/Å	23.2122(5)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	17239.8(11)
Z	9
ρ_{calc}g/cm^3	1.267
μ/mm^{-1}	1.001
F(000)	6912.0
Crystal color	colourless
Crystal size/mm^3	0.421 × 0.309 × 0.17
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.956 to 59.554
Index ranges	-38 ≤ h ≤ 40, -36 ≤ k ≤ 40, -31 ≤ l ≤ 31
Reflections collected	43023
Independent reflections	9623 [R_{int} = 0.0285, R_{sigma} = 0.0248]
Data/restraints/parameters	9623/3/399
Goodness-of-fit on F^2	1.116
Final R indexes [I>=2σ (I)]	R_1 = 0.0441, wR_2 = 0.0848
Final R indexes [all data]	R_1 = 0.0650, wR_2 = 0.0984

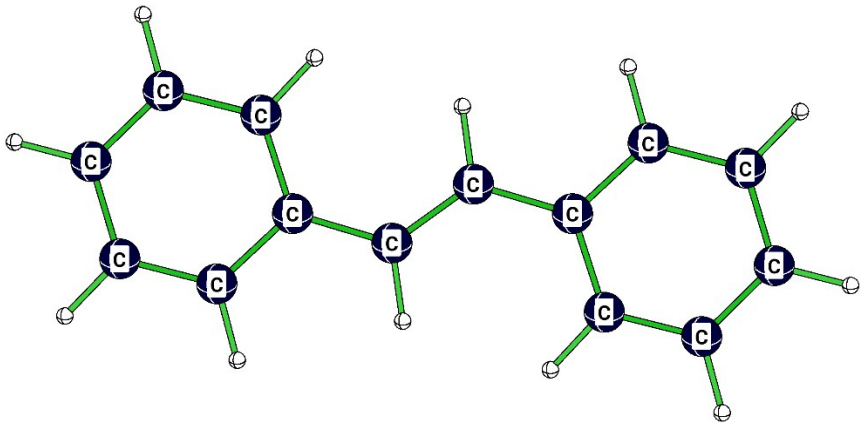
5. DFT calculations

General

All calculations were carried out using Gaussian 09 Rev.[5] D. All methods were used as implemented. All molecules were fully optimized on a B3PW91/6-311++G** level of theory.[6-10] All structures were determined to be true minima (NIMAG=0). Charges were determined via NBO-analysis.[11] Structures were drawn and evaluated using Molecule V2.3.[12] B3PW91-energies are given in Hartree, zero point energies (ZPE) are given in kcal/mol.

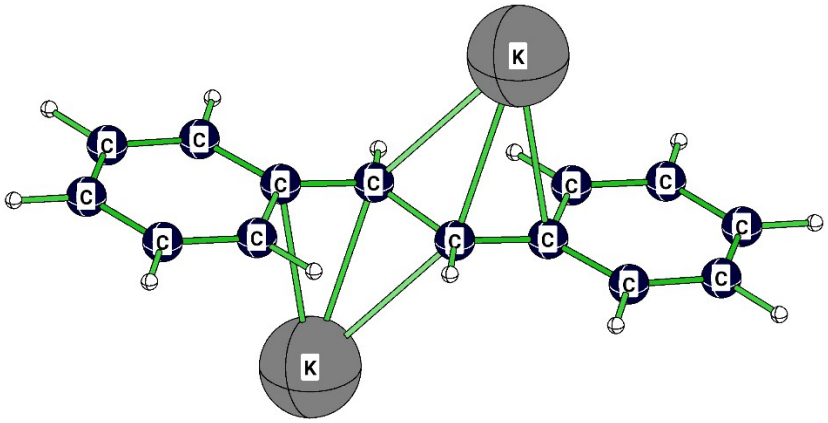
XYZ & NBO Charges

Stilbene dianion (SD^{2-})



B3PW91	-540.53326	ZPE	131.815	
	26			
SD				NPA-Charge
C	1.858005	1.843577	-0.776383	-0.255350
H	0.975706	2.447251	-0.586680	0.187260
C	3.010536	2.462199	-1.231508	-0.219700
H	3.004126	3.539916	-1.396944	0.122630
C	0.627141	-0.266166	-0.133290	-0.271760
C	1.796084	0.431838	-0.563803	-0.098790
C	3.019395	-0.269285	-0.774963	-0.224950
H	3.035807	-1.341882	-0.587373	0.178140
C	4.166990	0.357306	-1.225696	-0.239990
H	5.070648	-0.230428	-1.388091	0.068390
C	4.182393	1.737851	-1.481780	-0.336790
H	5.081910	2.231552	-1.839161	-0.084510
H	0.770817	-1.334135	0.029029	0.175420
C	-1.858005	-1.843577	0.776383	-0.255350
H	-0.975706	-2.447251	0.586680	0.187260
C	-3.010536	-2.462199	1.231508	-0.219700
H	-3.004126	-3.539916	1.396944	0.122630
C	-0.627141	0.266166	0.133290	-0.271760
C	-1.796084	-0.431838	0.563803	-0.098790
C	-3.019395	0.269285	0.774963	-0.224950
H	-3.035807	1.341882	0.587373	0.178140
C	-4.166990	-0.357306	1.225696	-0.239990
H	-5.070648	0.230428	1.388091	0.068390
C	-4.182393	-1.737851	1.481780	-0.336790
H	-5.081910	-2.231552	1.839161	-0.084510
H	-0.770817	1.334135	-0.029029	0.175420

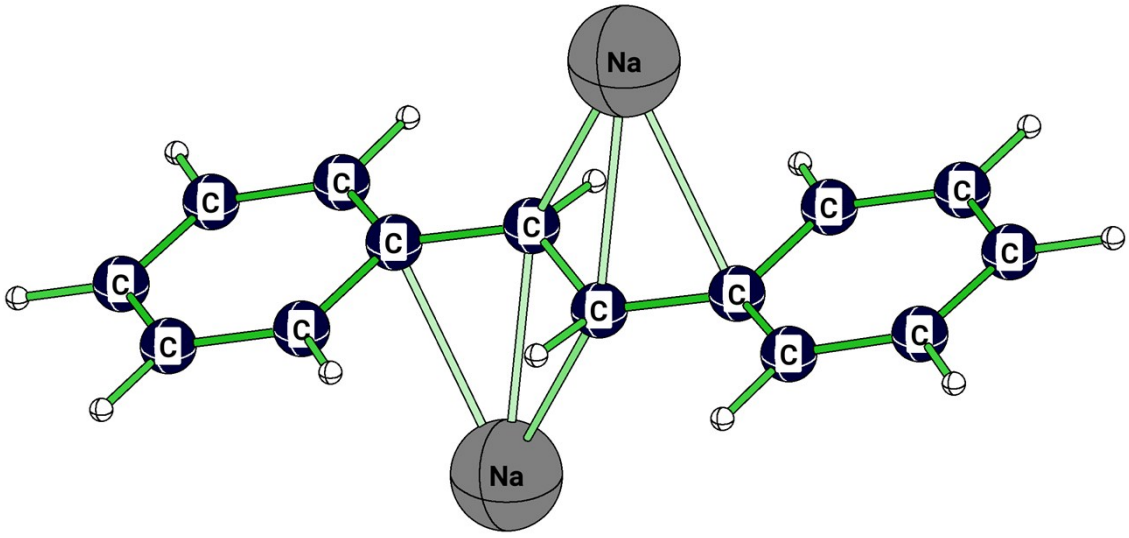
K_2(SD)



B3PW91 -1740.40436 ZPE 132.375

	28			
K				NPA-Charge
C	2.078713	-1.711892	-0.176816	-0.390820
C	-2.078713	1.711892	0.176816	-0.390820
H	1.486158	-1.949680	-1.056423	0.197730
H	-1.486158	1.949680	1.056423	0.197730
C	3.280704	-2.392777	0.018845	-0.188460
C	-3.280704	2.392777	-0.018845	-0.188460
H	3.609691	-3.094618	-0.745126	0.194950
H	-3.609691	3.094618	0.745126	0.194950
C	0.381994	-0.032912	0.620598	-0.558090
C	-0.381994	0.032912	-0.620598	-0.558090
C	1.554940	-0.799004	0.810500	-0.130040
C	-1.554940	0.799004	-0.810500	-0.130040
C	2.395819	-0.622659	1.964237	-0.265030
C	-2.395819	0.622659	-1.964237	-0.265030
H	2.061880	0.062447	2.741879	0.191720
H	-2.061880	-0.062447	-2.741879	0.191720
C	3.585536	-1.297106	2.126477	-0.209840
C	-3.585536	1.297106	-2.126477	-0.209840
H	4.169425	-1.123129	3.027385	0.196580
H	-4.169425	1.123129	-3.027385	0.196580
C	4.057608	-2.206575	1.156854	-0.339860
C	-4.057608	2.206575	-1.156854	-0.339860
H	4.990231	-2.741066	1.296345	0.200340
H	-4.990231	2.741066	-1.296345	0.200340
K	-2.187908	-1.148257	1.104962	0.905160
K	2.187908	1.148257	-1.104962	0.905160
H	0.197996	0.733609	1.374746	0.195660
H	-0.197996	-0.733609	-1.374746	0.195660

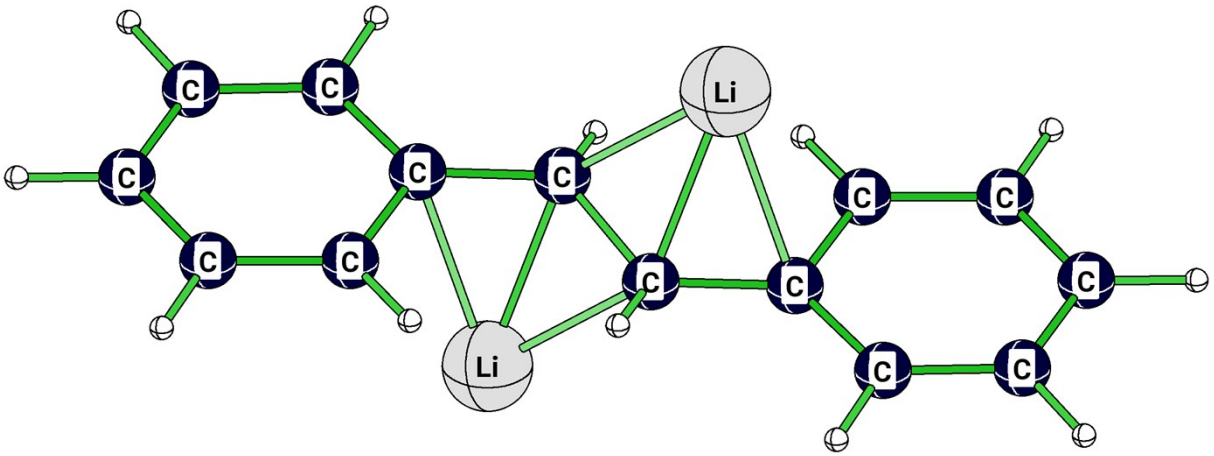
Na_2(SD)



B3PW91	-865.13510	ZPE	133.008

	28			
Na				NPA-Charge
C	2.093010	-1.681948	-0.190937	-0.381860
C	-2.093010	1.681948	0.190937	-0.381860
H	1.501512	-1.924132	-1.070181	0.203620
H	-1.501512	1.924132	1.070181	0.203620
C	3.302662	-2.358423	0.002469	-0.184910
C	-3.302662	2.358423	-0.002469	-0.184910
H	3.650182	-3.036895	-0.773069	0.199770
H	-3.650182	3.036895	0.773069	0.199770
C	0.348059	-0.066701	0.642473	-0.559890
C	-0.348059	0.066701	-0.642473	-0.559890
C	1.549636	-0.813714	0.816641	-0.118540
C	-1.549636	0.813714	-0.816641	-0.118540
C	2.369461	-0.645551	1.978298	-0.239870
C	-2.369461	0.645551	-1.978298	-0.239870
H	2.015589	0.018427	2.764171	0.196940
H	-2.015589	-0.018427	-2.764171	0.196940
C	3.565411	-1.307994	2.139985	-0.206690
C	-3.565411	1.307994	-2.139985	-0.206690
H	4.140031	-1.146668	3.048327	0.200860
H	-4.140031	1.146668	-3.048327	0.200860
C	4.054122	-2.189454	1.154463	-0.304880
C	-4.054122	2.189454	-1.154463	-0.304880
H	4.991064	-2.716531	1.294256	0.203580
H	-4.991064	2.716531	-1.294256	0.203580
Na	-1.956041	-0.798920	1.151103	0.790660
Na	1.956041	0.798920	-1.151103	0.790660
H	0.224879	0.746108	1.359778	0.201210
H	-0.224879	-0.746108	-1.359778	0.201210

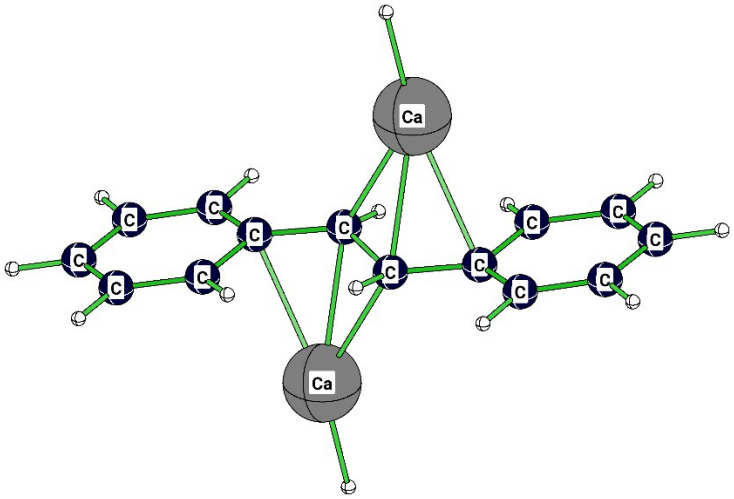
Li_2(SD)



B3PW91	-555.67706	ZPE	134.819

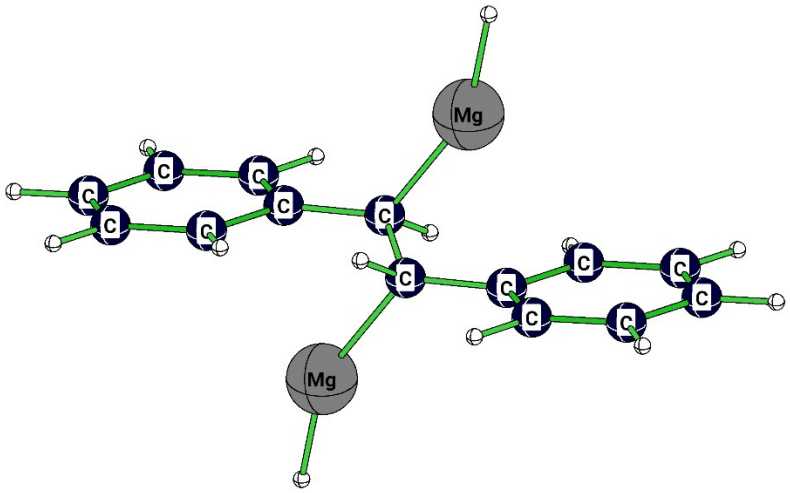
	28			
Li				NPA-Charge
C	2.075531	-1.664032	-0.180014	-0.397270
C	-2.075531	1.664032	0.180014	-0.397270
H	1.471998	-1.912938	-1.048688	0.213580
H	-1.471998	1.912938	1.048688	0.213580
C	3.295168	-2.334328	-0.007039	-0.171390
C	-3.295168	2.334328	0.007039	-0.171390
H	3.636084	-3.006067	-0.790543	0.202890
H	-3.636084	3.006067	0.790543	0.202890
C	0.358417	-0.026552	0.651432	-0.645150
C	-0.358417	0.026552	-0.651432	-0.645150
C	1.553621	-0.794872	0.834152	-0.127360
C	-1.553621	0.794872	-0.834152	-0.127360
C	2.371444	-0.646426	1.999174	-0.230450
C	-2.371444	0.646426	-1.999174	-0.230450
H	2.019175	0.005284	2.794965	0.201100
H	-2.019175	-0.005284	-2.794965	0.201100
C	3.566902	-1.309984	2.142106	-0.196720
C	-3.566902	1.309984	-2.142106	-0.196720
H	4.144520	-1.167217	3.051283	0.203560
H	-4.144520	1.167217	-3.051283	0.203560
C	4.055012	-2.168646	1.135796	-0.291610
C	-4.055012	2.168646	-1.135796	-0.291610
H	4.996114	-2.691569	1.261976	0.206040
H	-4.996114	2.691569	-1.261976	0.206040
Li	-1.661393	-0.523092	0.836776	0.809490
Li	1.661393	0.523092	-0.836776	0.809490
H	0.265833	0.835646	1.312225	0.223310
H	-0.265833	-0.835646	-1.312225	0.223310

$(HCa)_2$(SD)



B3PW91	-1896.90981 30	ZPE	138.323	
Ca				NPA-Charge
C	2.013964	-1.754228	-0.123634	-0.399540
C	-2.013964	1.754228	0.123634	-0.399540
H	1.386137	-2.026733	-0.968100	0.214580
H	-1.386137	2.026733	0.968100	0.214580
C	3.211856	-2.458695	0.063515	-0.167400
C	-3.211856	2.458695	-0.063515	-0.167400
H	3.513375	-3.184666	-0.686205	0.211190
H	-3.513375	3.184666	0.686205	0.211190
C	0.359919	-0.023892	0.650233	-0.694640
C	-0.359919	0.023892	-0.650233	-0.694640
C	1.537249	-0.822688	0.851633	-0.136320
C	-1.537249	0.822688	-0.851633	-0.136320
C	2.387173	-0.624463	1.981847	-0.240820
C	-2.387173	0.624463	-1.981847	-0.240820
H	2.077944	0.085447	2.744986	0.207840
H	-2.077944	-0.085447	-2.744986	0.207840
C	3.568989	-1.316721	2.137581	-0.180030
C	-3.568989	1.316721	-2.137581	-0.180030
H	4.174490	-1.133393	3.020191	0.211910
H	-4.174490	1.133393	-3.020191	0.211910
C	4.001959	-2.249978	1.179457	-0.271890
C	-4.001959	2.249978	-1.179457	-0.271890
H	4.929932	-2.792691	1.315085	0.213800
H	-4.929932	2.792691	-1.315085	0.213800
Ca	-2.014401	-0.908861	1.048602	1.512770
Ca	2.014401	0.908861	-1.048602	1.512770
H	0.282685	0.848882	1.301735	0.224100
H	-0.282685	-0.848882	-1.301735	0.224100
H	-3.026302	-2.481915	1.817676	-0.705570
H	3.026302	2.481915	-1.817676	-0.705570

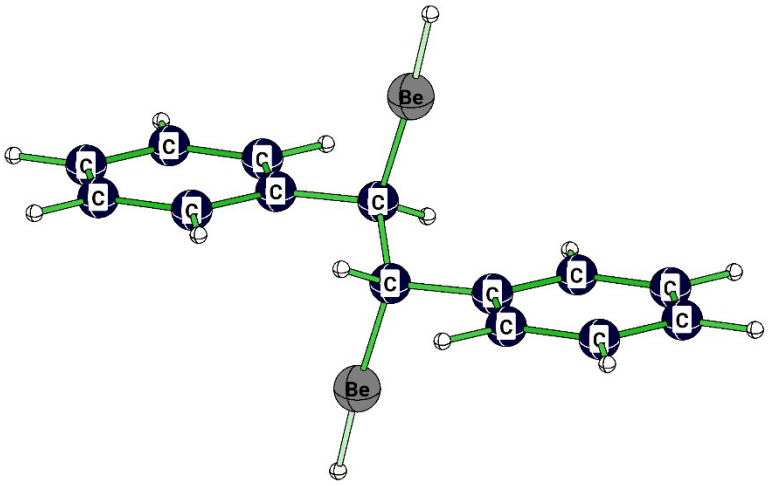
$(HMg)_2(SD)$



B3PW91	-941.89852	ZPE	140.888

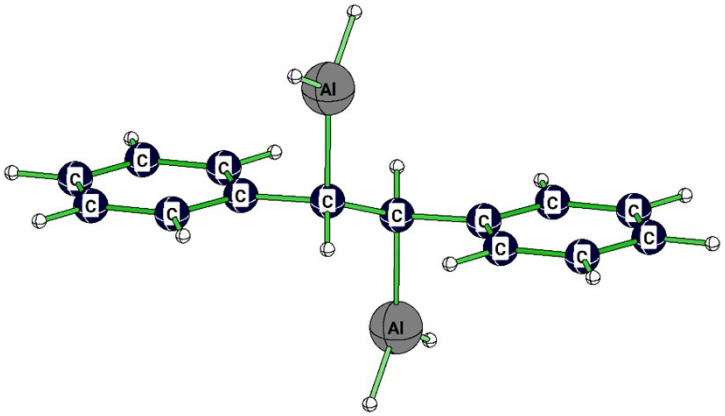
	30			
Mg				NPA-Charge
C	2.015749	-1.691752	-0.136807	-0.355550
C	-2.015749	1.691752	0.136807	-0.355550
H	1.392644	-1.942265	-0.990634	0.221920
H	-1.392644	1.942265	0.990634	0.221920
C	3.240692	-2.361181	0.010347	-0.170270
C	-3.240692	2.361181	-0.010347	-0.170270
H	3.568668	-3.038829	-0.771916	0.211450
H	-3.568668	3.038829	0.771916	0.211450
C	0.288943	-0.053688	0.713134	-0.758690
C	-0.288943	0.053688	-0.713134	-0.758690
C	1.530300	-0.817240	0.869639	-0.098990
C	-1.530300	0.817240	-0.869639	-0.098990
C	2.355152	-0.645037	2.009885	-0.208930
C	-2.355152	0.645037	-2.009885	-0.208930
H	2.020330	0.025785	2.796200	0.209330
H	-2.020330	-0.025785	-2.796200	0.209330
C	3.558110	-1.306027	2.139782	-0.180970
C	-3.558110	1.306027	-2.139782	-0.180970
H	4.159412	-1.146445	3.029500	0.211490
H	-4.159412	1.146445	-3.029500	0.211490
C	4.018138	-2.172947	1.136198	-0.238490
C	-4.018138	2.172947	-1.136198	-0.238490
H	4.965829	-2.687748	1.246800	0.212950
H	-4.965829	2.687748	-1.246800	0.212950
Mg	-1.728224	-0.758189	1.081069	1.265640
Mg	1.728224	0.758189	-1.081069	1.265640
H	0.356019	0.907984	1.233617	0.227020
H	-0.356019	-0.907984	-1.233617	0.227020
H	-2.942531	-1.895569	1.461108	-0.547910
H	2.942531	1.895569	-1.461108	-0.547910

$(HBe)_2(SD)$



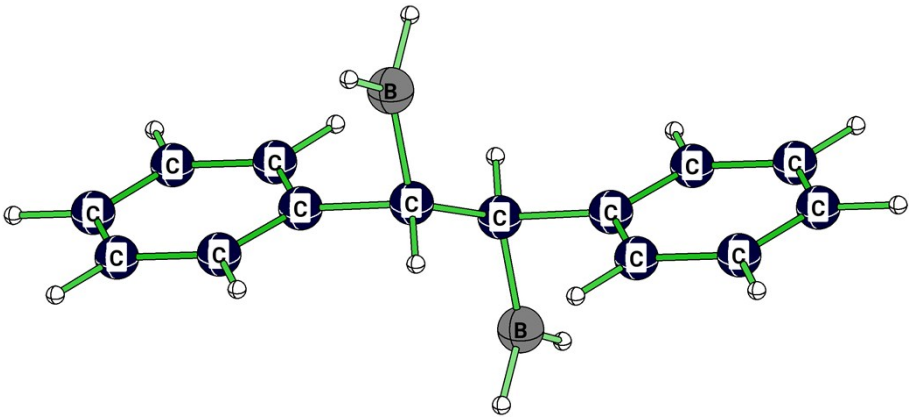
B3PW91	-571.28545	ZPE	145.207	
	30			
Be				NPA-Charge
C	2.014055	-1.772065	-0.092046	-0.243200
C	-2.014055	1.772065	0.092046	-0.243200
H	1.447978	-1.952006	-1.000231	0.206570
H	-1.447978	1.952006	1.000231	0.206570
C	3.222529	-2.443791	0.086804	-0.189380
C	-3.222529	2.443791	-0.086804	-0.189380
H	3.575635	-3.120732	-0.684997	0.208640
H	-3.575635	3.120732	0.684997	0.208640
C	0.204782	-0.173516	0.737499	-0.853080
C	-0.204782	0.173516	-0.737499	-0.853080
C	1.523068	-0.887681	0.879554	-0.038520
C	-1.523068	0.887681	-0.879554	-0.038520
C	2.297618	-0.708265	2.037696	-0.215080
C	-2.297618	0.708265	-2.037696	-0.215080
H	1.948079	-0.023009	2.805825	0.205280
H	-1.948079	0.023009	-2.805825	0.205280
C	3.499567	-1.377992	2.217382	-0.191630
C	-3.499567	1.377992	-2.217382	-0.191630
H	4.075903	-1.212010	3.122262	0.209340
H	-4.075903	1.212010	-3.122262	0.209340
C	3.971960	-2.252717	1.240151	-0.223710
C	-3.971960	2.252717	-1.240151	-0.223710
H	4.912936	-2.774542	1.377777	0.210170
H	-4.912936	2.774542	-1.377777	0.210170
Be	-1.046363	-1.166732	1.314374	1.151890
Be	1.046363	1.166732	-1.314374	1.151890
H	0.264427	0.745710	1.333422	0.231170
H	-0.264427	-0.745710	-1.333422	0.231170
H	-1.992793	-2.022323	1.703711	-0.468460
H	1.992793	2.022323	-1.703711	-0.468460

$(H_2Al)_2$(SD)



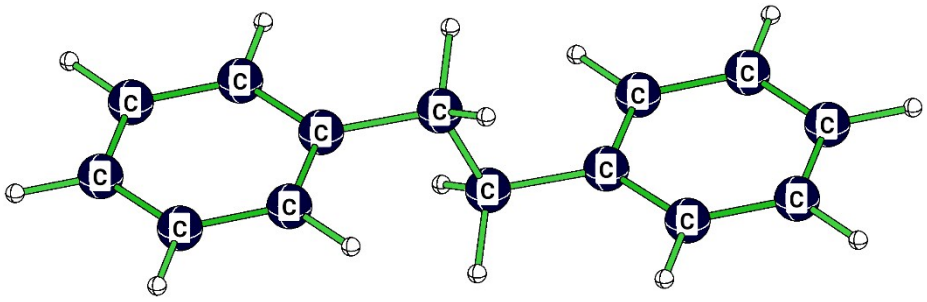
B3PW91	-1027.81879	ZPE	152.224	
	32			
Al				NPA-Charge
C	-2.439618	-0.705219	-0.865050	-0.236050
C	2.439757	0.705048	0.865222	-0.236030
H	-1.751535	-1.155562	-1.572263	0.213420
H	1.751717	1.155288	1.572542	0.213410
C	-3.800339	-0.977485	-0.983482	-0.190770
C	3.800496	0.977185	0.983687	-0.190780
H	-4.144493	-1.638112	-1.773176	0.210580
H	4.144715	1.637634	1.773501	0.210580
C	-0.501036	0.507216	0.275401	-0.763590
C	0.501066	-0.507016	-0.275471	-0.763590
C	-1.952251	0.137793	0.149506	-0.073640
C	1.952308	-0.137715	-0.149500	-0.073630
C	-2.897924	0.704257	1.027765	-0.217320
C	2.897927	-0.704117	-1.027856	-0.217320
H	-2.551893	1.353290	1.827935	0.213610
H	2.551829	-1.352993	-1.828123	0.213610
C	-4.253649	0.434016	0.904261	-0.193290
C	4.253681	-0.434023	-0.904308	-0.193300
H	-4.954050	0.879159	1.603875	0.211770
H	4.954041	-0.879114	-1.603994	0.211770
C	-4.714672	-0.411528	-0.102917	-0.218990
C	4.714776	0.411314	0.103006	-0.218990
H	-5.773731	-0.626160	-0.197589	0.211530
H	5.773853	0.625845	0.197709	0.211520
Al	-0.616609	2.204238	-0.765979	1.344000
Al	0.616377	-2.204095	0.765852	1.344010
H	-0.304817	0.731705	1.328345	0.236660
H	0.304874	-0.731441	-1.328436	0.236650
H	-0.472852	2.097983	-2.344938	-0.372620
H	0.472593	-2.097844	2.344809	-0.372620
H	-0.986133	3.575378	-0.049222	-0.375300
H	0.985766	-3.575265	0.049081	-0.375300

$(H_2B)_2$(SD)



B3PW91	-592.68649	ZPE	162.235	
	32			
B				NPA-Charge
C	-2.638712	0.567471	0.241855	-0.096730
C	2.638712	-0.567471	-0.241855	-0.096730
H	-2.434571	0.710541	-0.813220	0.107590
H	2.434571	-0.710541	0.813220	0.107590
C	-3.955638	0.602352	0.689648	-0.100620
C	3.955638	-0.602352	-0.689648	-0.100620
H	-4.759091	0.771433	-0.020008	0.105650
H	4.759091	-0.771433	0.020008	0.105650
C	-0.123798	0.331983	0.678667	-0.282790
C	0.123798	-0.331983	-0.678667	-0.282790
C	-1.580761	0.334317	1.132879	-0.021570
C	1.580761	-0.334317	-1.132879	-0.021570
C	-1.889229	0.180350	2.494188	-0.090910
C	1.889229	-0.180350	-2.494188	-0.090910
H	-1.082100	0.016595	3.202044	0.106140
H	1.082100	-0.016595	-3.202044	0.106140
C	-3.202347	0.216294	2.941149	-0.100800
C	3.202347	-0.216294	-2.941149	-0.100800
H	-3.416318	0.078934	3.996189	0.105940
H	3.416318	-0.078934	-3.996189	0.105940
C	-4.242805	0.424645	2.038201	-0.098720
C	4.242805	-0.424645	-2.038201	-0.098720
H	-5.270301	0.450474	2.386010	0.105480
H	5.270301	-0.450474	-2.386010	0.105480
B	-0.060364	1.892716	0.766443	0.223000
B	0.060364	-1.892716	-0.766443	0.223000
H	0.447266	-0.168589	1.463872	0.114720
H	-0.447266	0.168589	-1.463872	0.114720
H	-0.347681	2.548913	-0.193125	-0.039030
H	0.347681	-2.548913	0.193125	-0.039030
H	0.183428	2.436857	1.802993	-0.037360
H	-0.183428	-2.436857	-1.802993	-0.037360

H_2(SD) - diphenylethane



B3PW91	9541.85228	ZPE	149.079	
	28			
H				NPA-Charge
C	-2.792561	0.711486	0.110738	-0.206580
C	2.792561	-0.711486	-0.110738	-0.206580
H	-2.659073	1.118010	-0.888315	0.205310
H	2.659073	-1.118010	0.888315	0.205310
C	-4.077351	0.490950	0.597567	-0.201390
C	4.077351	-0.490950	-0.597567	-0.201390
H	-4.936956	0.723960	-0.023066	0.207940
H	4.936956	-0.723960	0.023066	0.207940
C	-0.278120	0.630956	0.346487	-0.395750
C	0.278120	-0.630956	-0.346487	-0.395750
C	-1.668640	0.427378	0.890513	-0.030480
C	1.668640	-0.427378	-0.890513	-0.030480
C	-1.868003	-0.083764	2.175821	-0.206600
C	1.868003	0.083764	-2.175821	-0.206600
H	-1.007180	-0.303078	2.802049	0.205330
H	1.007180	0.303078	-2.802049	0.205330
C	-3.150232	-0.306493	2.667668	-0.201400
C	3.150232	0.306493	-2.667668	-0.201400
H	-3.282834	-0.699428	3.670863	0.207920
H	3.282834	0.699428	-3.670863	0.207920
C	-4.260595	-0.020486	1.878724	-0.214980
C	4.260595	0.020486	-1.878724	-0.214980
H	-5.261658	-0.189994	2.261700	0.208720
H	5.261658	0.189994	-2.261700	0.208720
H	0.401089	0.919065	1.155953	0.211270
H	-0.401089	-0.919065	-1.155953	0.211270
H	-0.276228	1.458954	-0.370275	0.210700
H	0.276228	-1.458954	0.370275	0.210700

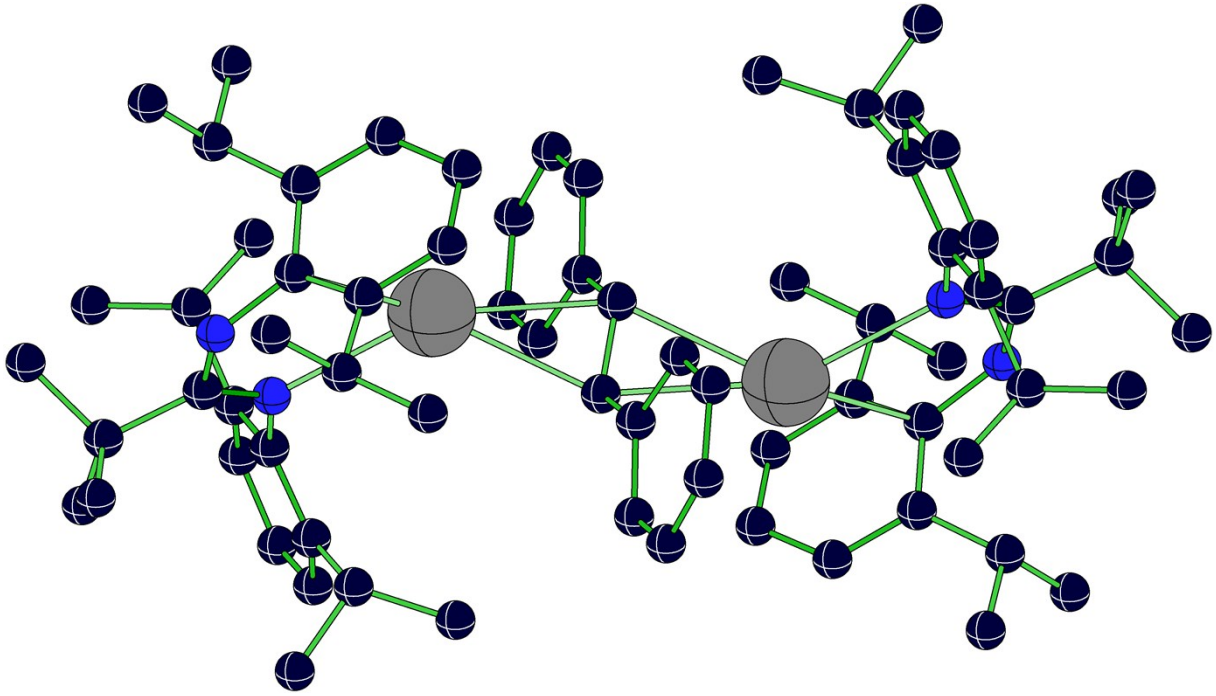
Full optimization of complex 2

Complex **2** was optimized on B3LYP/6-311G* [13] and B3PW91/6-311+G** levels of theory. The C_i symmetry was maintained. The structure was determined to be a true minimum by frequency analysis (NIMAG=0) at the B3LYP/6-311G* level and the ZPE was determined. Charges were determined by the NPA method.[11] The calculated bond lengths compare reasonably well with those in the crystal structure and those in the smaller model system. Largest differences are found for the M-C bond distances. The geometry of the stilbene dianion is remarkably similar. Also the NPA charges compare reasonably well.

NPA Charges Part/Atom	**Complex 2 B3LYP/6-311G***	**Complex 2 B3PW91/6-311+G****	**$(HCa)_2SD$ B3PW91/6-311++G****
Ca	+1.445	+1.365	+1.513
Ligand or H^-	-0.737	-0.685	-0.706
Ph (Stilbene)	-0.343	-0.329	-0.337
CH (Stilbene), C, H	-0.365, -0.584, +0.219	-0.351, -0.589, +0.238	-0.471, -0.695, 0.224
Stilbene total	-1.415	-1.361	-1.614

Bond	**Complex 2 crystal**	**Complex 2 B3LYP/6-311G***	**Complex 2 B3PW91/6-311+G****	**$(HCa)_2SD$**
Ca-C1	2.591	2.649	2.631	2.548
Ca-C2	2.616	2.678	2.675	2.565
C1=C2	1.453	1.466	1.459	1.487
C-Ph	1.437	1.435	1.431	1.437

B3LYP/6-311G*



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Complex 2	B3LYP=-4378.78606		ZPE=971.035
N	-3.339925	-3.344104	3.291623
H	-3.410412	-4.182634	3.849291
N	-3.418200	-1.053790	3.301735
C	-3.695079	-2.178741	3.917425
C	-3.769006	0.252175	3.764122
C	-2.799381	1.040488	4.438352
C	-4.377271	-2.450030	5.299497
C	-1.420406	-3.778087	1.773779
C	-2.811976	-3.443792	1.974899
C	-0.610230	-4.324598	2.941560
C	-3.705147	-3.299876	0.825479
C	-5.031474	0.816405	3.442477
C	2.118917	-1.664074	-0.198858
H	1.540131	-1.885569	-1.089761
C	-3.132538	2.345142	4.814531
H	-2.402675	2.945998	5.347732
C	-5.203476	-3.494484	0.999929
H	-5.512791	-2.963654	1.906891
C	-5.304348	2.128700	3.834036
H	-6.270156	2.561546	3.593175
C	-0.892537	-3.633155	0.501627
C	-4.797977	-1.206569	6.102563
H	-3.966087	-0.549216	6.342446
H	-5.231308	-1.545594	7.048285

H	-5.550854	-0.609659	5.595180
C	-6.107240	0.052268	2.673103
H	-5.753195	-0.969543	2.532617
C	-4.373533	2.893615	4.524865
H	-4.610062	3.909022	4.826701
C	-3.118571	-3.183446	-0.426449
C	3.293266	-2.394388	0.018438
H	3.624927	-3.084655	-0.751919
C	-3.384896	-3.245210	6.190350
H	-3.153021	-4.241698	5.806715
H	-3.819855	-3.385390	7.183247
H	-2.440469	-2.710353	6.312826
C	0.375526	-0.035085	0.628378
C	1.593937	-0.774092	0.793635
C	-1.713252	-3.232996	-0.602268
C	-6.331792	0.652658	1.274076
H	-6.701905	1.680467	1.339436
H	-7.074382	0.070268	0.720397
H	-5.413006	0.676877	0.687033
C	-1.401423	0.523342	4.780222
C	2.421855	-0.595679	1.949208
H	2.100060	0.110365	2.709162
C	-5.653350	-3.301080	5.082879
H	-6.376798	-2.778241	4.453609
H	-6.132680	-3.493987	6.047551
H	-5.450220	-4.267697	4.619151
C	-5.516428	-4.988226	1.232659
H	-5.270772	-5.575778	0.343170
H	-6.578549	-5.136507	1.454988
H	-4.938672	-5.396326	2.065050
C	3.585431	-1.313601	2.138512
H	4.161460	-1.155253	3.046438
C	4.033098	-2.245313	1.182857
H	4.944022	-2.811018	1.342923
C	-0.297970	1.471229	4.276495
H	-0.415396	1.705448	3.217332
H	0.687160	1.017564	4.414778
H	-0.298309	2.418155	4.822921
C	-6.057233	-2.958388	-0.155788
H	-5.829320	-1.914643	-0.382635
H	-7.118860	-3.022157	0.099752
H	-5.914740	-3.540622	-1.070856
C	-1.016628	-5.787277	3.224729
H	-2.094005	-5.903455	3.375152
H	-0.510910	-6.166798	4.118202

H	-0.742143	-6.428915	2.382509
C	-7.449849	-0.017082	3.425985
H	-7.346876	-0.438641	4.428168
H	-8.161331	-0.639798	2.875101
H	-7.903750	0.971869	3.534047
C	0.910514	-4.232779	2.776254
H	1.271957	-4.889653	1.980412
H	1.404774	-4.547760	3.700077
C	-1.204417	0.285018	6.289970
H	-1.333837	1.212383	6.855720
H	-0.194540	-0.086089	6.490505
H	-1.909074	-0.444432	6.691328
Ca	-2.018972	-1.143718	1.083084
H	0.242723	0.779061	1.335294
H	0.156684	-3.836252	0.326975
H	-1.287306	-3.148490	-1.593406
H	-3.747982	-3.071271	-1.302885
H	-0.880733	-3.737014	3.829151
H	-1.268491	-0.439407	4.278721
H	1.245258	-3.220077	2.547550
C	-2.118917	1.664074	0.198858
H	-1.540131	1.885569	1.089761
C	-3.293266	2.394388	-0.018438
H	-3.624927	3.084655	0.751919
C	-0.375526	0.035085	-0.628378
C	-1.593937	0.774092	-0.793635
C	-2.421855	0.595679	-1.949208
H	-2.100060	-0.110365	-2.709162
C	-3.585431	1.313601	-2.138512
H	-4.161460	1.155253	-3.046438
C	-4.033098	2.245313	-1.182857
H	-4.944022	2.811018	-1.342923
H	-0.242723	-0.779061	-1.335294
N	3.339925	3.344104	-3.291623
H	3.410412	4.182634	-3.849291
N	3.418200	1.053790	-3.301735
C	3.695079	2.178741	-3.917425
C	3.769006	-0.252175	-3.764122
C	2.799381	-1.040488	-4.438352
C	4.377271	2.450030	-5.299497
C	1.420406	3.778087	-1.773779
C	2.811976	3.443792	-1.974899
C	0.610230	4.324598	-2.941560
C	3.705147	3.299876	-0.825479
C	5.031474	-0.816405	-3.442477

C	3.132538	-2.345142	-4.814531
H	2.402675	-2.945998	-5.347732
C	5.203476	3.494484	-0.999929
H	5.512791	2.963654	-1.906891
C	5.304348	-2.128700	-3.834036
H	6.270156	-2.561546	-3.593175
C	0.892537	3.633155	-0.501627
C	4.797977	1.206569	-6.102563
H	3.966087	0.549216	-6.342446
H	5.231308	1.545594	-7.048285
H	5.550854	0.609659	-5.595180
C	6.107240	-0.052268	-2.673103
H	5.753195	0.969543	-2.532617
C	4.373533	-2.893615	-4.524865
H	4.610062	-3.909022	-4.826701
C	3.118571	3.183446	0.426449
C	3.384896	3.245210	-6.190350
H	3.153021	4.241698	-5.806715
H	3.819855	3.385390	-7.183247
H	2.440469	2.710353	-6.312826
C	1.713252	3.232996	0.602268
C	6.331792	-0.652658	-1.274076
H	6.701905	-1.680467	-1.339436
H	7.074382	-0.070268	-0.720397
H	5.413006	-0.676877	-0.687033
C	1.401423	-0.523342	-4.780222
C	5.653350	3.301080	-5.082879
H	6.376798	2.778241	-4.453609
H	6.132680	3.493987	-6.047551
H	5.450220	4.267697	-4.619151
C	5.516428	4.988226	-1.232659
H	5.270772	5.575778	-0.343170
H	6.578549	5.136507	-1.454988
H	4.938672	5.396326	-2.065050
C	0.297970	-1.471229	-4.276495
H	0.415396	-1.705448	-3.217332
H	-0.687160	-1.017564	-4.414778
H	0.298309	-2.418155	-4.822921
C	6.057233	2.958388	0.155788
H	5.829320	1.914643	0.382635
H	7.118860	3.022157	-0.099752
H	5.914740	3.540622	1.070856
C	1.016628	5.787277	-3.224729
H	2.094005	5.903455	-3.375152
H	0.510910	6.166798	-4.118202

H	0.742143	6.428915	-2.382509
C	7.449849	0.017082	-3.425985
H	7.346876	0.438641	-4.428168
H	8.161331	0.639798	-2.875101
H	7.903750	-0.971869	-3.534047
C	-0.910514	4.232779	-2.776254
H	-1.271957	4.889653	-1.980412
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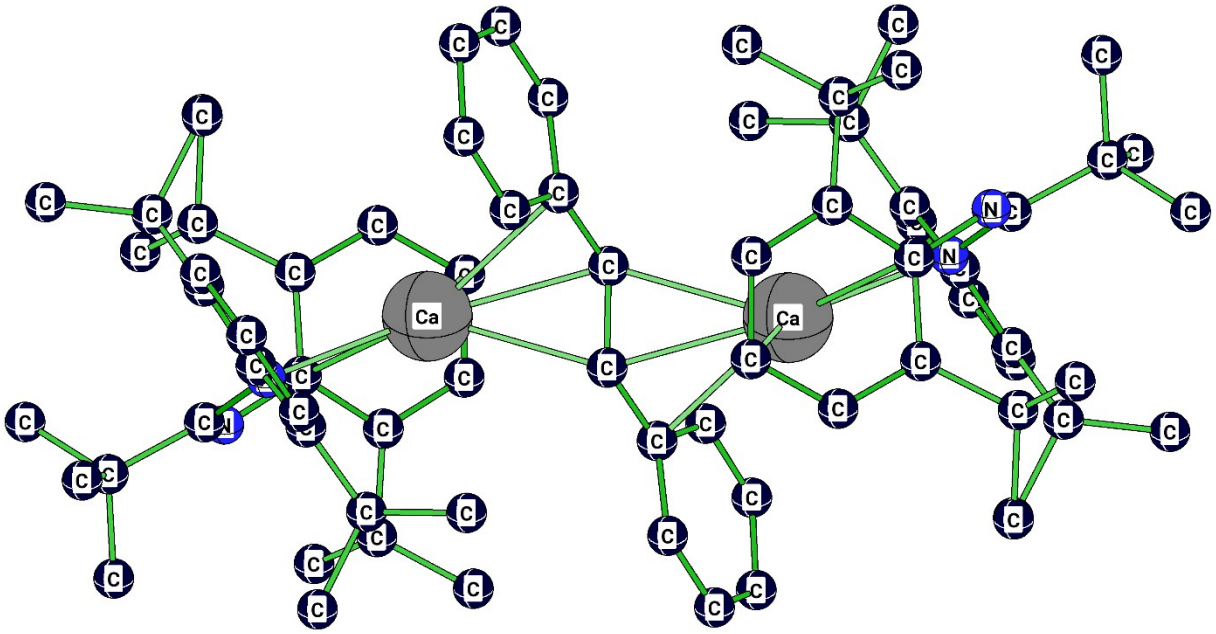
C	1.204417	-0.285018	-6.289970
H	1.333837	-1.212383	-6.855720
H	0.194540	0.086089	-6.490505
H	1.909074	0.444432	-6.691328
Ca	2.018972	1.143718	-1.083084
H	-0.156684	3.836252	-0.326975
H	1.287306	3.148490	1.593406
H	3.747982	3.071271	1.302885
H	0.880733	3.737014	-3.829151
H	1.268491	0.439407	-4.278721
H	-1.245258	3.220077	-2.547550

B3PW91/6-311+G**



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N	-3.422137	-1.050277	3.290195
C	-3.701523	-2.172126	3.906836
C	-3.770115	0.247037	3.755351
C	-2.789329	1.036500	4.406786
C	-4.402675	-2.440188	5.269261
C	-1.405370	-3.732390	1.790500
C	-2.796271	-3.422362	1.983041
C	-0.598562	-4.262888	2.960525
C	-3.679137	-3.263010	0.831840
C	-5.039766	0.806967	3.467538
C	2.123076	-1.640436	-0.211518
H	1.540988	-1.858588	-1.102260
C	-3.119529	2.333721	4.802156
H	-2.378355	2.933362	5.321404
C	-5.171986	-3.459959	0.997291
H	-5.486882	-2.924392	1.901142
C	-5.310260	2.112941	3.873557
H	-6.284363	2.540606	3.656756
C	-0.866041	-3.575059	0.524941
C	-4.784831	-1.197820	6.082022
H	-3.929929	-0.569082	6.325919
H	-5.229067	-1.536971	7.023659
H	-5.517382	-0.572825	5.575938
C	-6.122317	0.044704	2.718709

H	-5.774675	-0.983027	2.593086
C	-4.369160	2.877067	4.548453
H	-4.604058	3.888215	4.864725
C	-3.086118	-3.142205	-0.415518
C	3.301640	-2.362163	-0.002842
H	3.632626	-3.050912	-0.774797
C	-3.456312	-3.282304	6.157137
H	-3.258858	-4.283244	5.762783
H	-3.916129	-3.417942	7.140276
H	-2.494546	-2.783940	6.301539
C	0.381480	-0.023902	0.621122
C	1.600086	-0.756525	0.783827
C	-1.683435	-3.188334	-0.585085
C	-6.342512	0.631057	1.319048
H	-6.698426	1.664791	1.382111
H	-7.095992	0.053415	0.774455
H	-5.423040	0.637930	0.730526
C	-1.387027	0.522430	4.706692
C	2.431496	-0.572165	1.931976
H	2.108735	0.132037	2.693125
C	-5.696819	-3.242872	5.019822
H	-6.395907	-2.681087	4.395552
H	-6.190055	-3.443531	5.976947
H	-5.510034	-4.202452	4.532740
C	-5.476525	-4.949672	1.233325
H	-5.219904	-5.535642	0.344999
H	-6.539782	-5.102598	1.448503
H	-4.899093	-5.349545	2.070714
C	3.599324	-1.282068	2.113519
H	4.180718	-1.118956	3.017038
C	4.046452	-2.209514	1.156416
H	4.960124	-2.771634	1.311919
C	-0.304052	1.510130	4.256203
H	-0.434392	1.809122	3.213930
H	0.687081	1.060370	4.362652
H	-0.313662	2.420459	4.862942
C	-6.010768	-2.935935	-0.167343
H	-5.780525	-1.892760	-0.397420
H	-7.075353	-3.003387	0.076163
H	-5.851453	-3.527035	-1.074978
C	-0.984983	-5.727235	3.232909
H	-2.063018	-5.857613	3.369444
H	-0.481489	-6.101620	4.130187
H	-0.690523	-6.358737	2.388839
C	-7.457680	0.003030	3.474945

H	-7.354675	-0.403877	4.484038
H	-8.177887	-0.619033	2.933835
H	-7.897002	1.000934	3.566908
C	0.915281	-4.145609	2.802066
H	1.286699	-4.795589	2.004228
H	1.410919	-4.455841	3.727160
C	-1.181067	0.200789	6.193966
H	-1.337644	1.092751	6.809287
H	-0.159989	-0.152660	6.370716
H	-1.866290	-0.570748	6.549365
Ca	-2.007645	-1.130866	1.094245
H	0.231493	0.777379	1.341020
H	0.188295	-3.764676	0.363345
H	-1.254169	-3.102323	-1.574471
H	-3.714600	-3.025479	-1.292485
H	-0.889504	-3.679499	3.845085
H	-1.249421	-0.409758	4.148675
H	1.230446	-3.124752	2.575786
C	-2.123076	1.640436	0.211518
H	-1.540988	1.858588	1.102260
C	-3.301640	2.362163	0.002842
H	-3.632626	3.050912	0.774797
C	-0.381480	0.023902	-0.621122
C	-1.600086	0.756525	-0.783827
C	-2.431496	0.572165	-1.931976
H	-2.108735	-0.132037	-2.693125
C	-3.599324	1.282068	-2.113519
H	-4.180718	1.118956	-3.017038
C	-4.046452	2.209514	-1.156416
H	-4.960124	2.771634	-1.311919
H	-0.231493	-0.777379	-1.341020
N	3.332356	3.332889	-3.290157
H	3.399998	4.170538	-3.849726
N	3.422137	1.050277	-3.290195
C	3.701523	2.172126	-3.906836
C	3.770115	-0.247037	-3.755351
C	2.789329	-1.036500	-4.406786
C	4.402675	2.440188	-5.269261
C	1.405370	3.732390	-1.790500
C	2.796271	3.422362	-1.983041
C	0.598562	4.262888	-2.960525
C	3.679137	3.263010	-0.831840
C	5.039766	-0.806967	-3.467538
C	3.119529	-2.333721	-4.802156
H	2.378355	-2.933362	-5.321404

C	5.171986	3.459959	-0.997291
H	5.486882	2.924392	-1.901142
C	5.310260	-2.112941	-3.873557
H	6.284363	-2.540606	-3.656756
C	0.866041	3.575059	-0.524941
C	4.784831	1.197820	-6.082022
H	3.929929	0.569082	-6.325919
H	5.229067	1.536971	-7.023659
H	5.517382	0.572825	-5.575938
C	6.122317	-0.044704	-2.718709
H	5.774675	0.983027	-2.593086
C	4.369160	-2.877067	-4.548453
H	4.604058	-3.888215	-4.864725
C	3.086118	3.142205	0.415518
C	3.456312	3.282304	-6.157137
H	3.258858	4.283244	-5.762783
H	3.916129	3.417942	-7.140276
H	2.494546	2.783940	-6.301539
C	1.683435	3.188334	0.585085
C	6.342512	-0.631057	-1.319048
H	6.698426	-1.664791	-1.382111
H	7.095992	-0.053415	-0.774455
H	5.423040	-0.637930	-0.730526
C	1.387027	-0.522430	-4.706692
C	5.696819	3.242872	-5.019822
H	6.395907	2.681087	-4.395552
H	6.190055	3.443531	-5.976947
H	5.510034	4.202452	-4.532740
C	5.476525	4.949672	-1.233325
H	5.219904	5.535642	-0.344999
H	6.539782	5.102598	-1.448503
H	4.899093	5.349545	-2.070714
C	0.304052	-1.510130	-4.256203
H	0.434392	-1.809122	-3.213930
H	-0.687081	-1.060370	-4.362652
H	0.313662	-2.420459	-4.862942
C	6.010768	2.935935	0.167343
H	5.780525	1.892760	0.397420
H	7.075353	3.003387	-0.076163
H	5.851453	3.527035	1.074978
C	0.984983	5.727235	-3.232909
H	2.063018	5.857613	-3.369444
H	0.481489	6.101620	-4.130187
H	0.690523	6.358737	-2.388839
C	7.457680	-0.003030	-3.474945

H	7.354675	0.403877	-4.484038
H	8.177887	0.619033	-2.933835
H	7.897002	-1.000934	-3.566908
C	-0.915281	4.145609	-2.802066
H	-1.286699	4.795589	-2.004228
H	-1.410919	4.455841	-3.727160
C	1.181067	-0.200789	-6.193966
H	1.337644	-1.092751	-6.809287
H	0.159989	0.152660	-6.370716
H	1.866290	0.570748	-6.549365
Ca	2.007645	1.130866	-1.094245
H	-0.188295	3.764676	-0.363345
H	1.254169	3.102323	1.574471
H	3.714600	3.025479	1.292485
H	0.889504	3.679499	-3.845085
H	1.249421	0.409758	-4.148675
H	-1.230446	3.124752	-2.575786

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