Electronic Supplementary Material (ESI) for ChemComm.


## Supplementary Information

# Large Decanuclear Calcium and Strontium Hydride Clusters

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# 1 General Experimental Procedures

All air- and moisture-sensitive manipulations were carried out in dry glassware under an atmosphere of $N_2$ using standard Schlenk techniques or in a glovebox (MBraun, Labmaster SP). Benzene, hexanes, *n*-pentane and toluene were degassed with $N_2$, dried over activated aluminum oxide (Solvent Purification System: Pure Solv 400−4−MD, Innovative Technology) and stored over molecular sieves (3 Å) under an inert atmosphere.

$Ca[N(DIPP)(Si^iPr_3)]_2$ and $Sr[N(DIPP)(Si^iPr_3)]_2$ were prepared according to previously reported procedures.[1] *N,N,N′,N′′,N′′*-Pentamethyldiethylenetriamine (PMDTA; Alfa Aesar, 98%) was dried by stirring over freshly ground $CaH_2$ at room temperature overnight, distilled under reduced pressure and stored in a $N_2$-filled glovebox over molecular sieves (3 Å) prior to use. Phenylsilane ($PhSiH_3$; 97%) was purchased from Alfa Aesar and used as received.

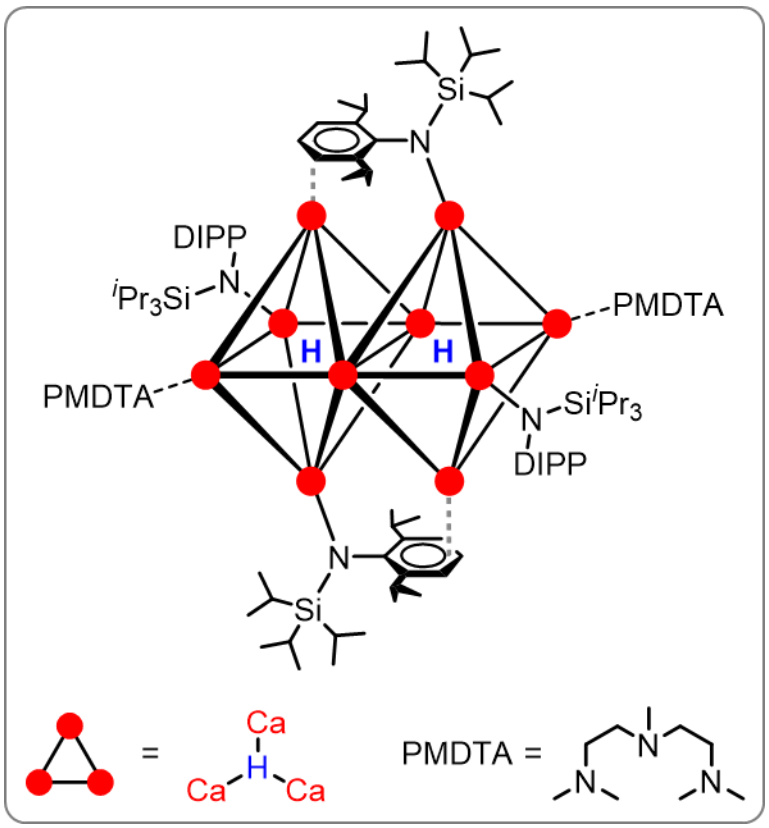
Infrared spectra were acquired on a Bruker Alpha II FT-IR spectrometer equipped with a Platinum ATR diamond from crystalline samples under inert conditions inside a glovebox. All spectra were recorded at room temperature in the range of 400 – 4000 $cm^{-1}$ with a resolution of 4 $cm^{-1}$ and baseline corrected. Wavenumbers are given in $cm^{-1}$ and intensities of IR bands are described using the following terms: s = strong, m = medium and w = weak.

Elemental analyses were performed with a HEKAtech Euro Vector EA3000 analyzer. Melting points were determined in sealed glass capillaries under $N_2$ with a Stuart melting point apparatus SMP10 and are uncorrected.

Both crystal structures have been measured on a SuperNova (Agilent) diffractometer with a dual Cu and Mo microfocus and an Atlas S2 detector. Crystallographic data have been deposited with The Cambridge Crystallographic Data Centre as supplementary publication numbers CCDC 1970934 (for $Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$) and CCDC 1970936 (for $Sr_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$).

# 2 Synthetic and Analytical Data for $Ae_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$

**Synthesis of $Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (1)**




This complex was prepared by three slightly different methods:

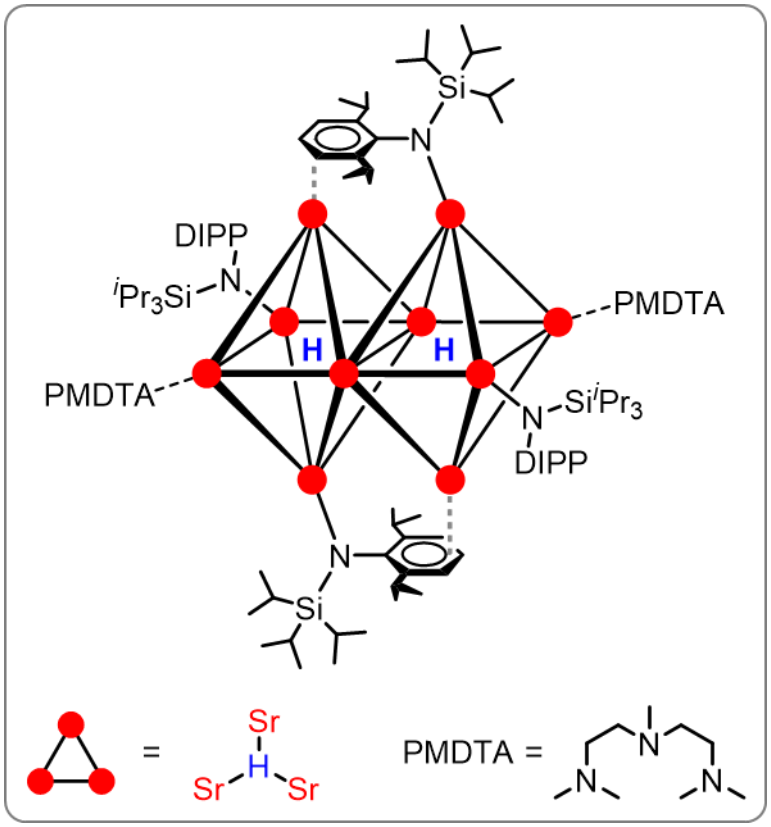
*Method A:* To a solution of $Ca[N(DIPP)(Si^iPr_3)]_2$ (91 mg, 0.129 mmol) in toluene (0.7 mL) were sequentially added $PhSiH_3$ (25.5 µL, 22.4 mg, 0.207 mmol, 1.6 eq.) and PMDTA (26.9 µL, 22.3 mg, 0.129 mmol, 1 eq.) with gentle shaking to afford a slightly turbid, colorless solution. Hexanes (3 mL reservoir) was then allowed to slowly diffuse into the reaction mixture *via* the gas phase at room temperature in a sealed vessel over the course of three days, resulting in the deposition of $Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (17 mg, 8.1 µmol, 63%) as well-defined, needle-shaped crystals suitable for X-ray diffraction analysis. The supernatant reaction solution was decanted, and the colorless crystals formed were washed multiple times with cold pentane (−20 °C; 3 × 1 mL), dried extensively *in vacuo* at ambient temperature to remove residual volatile components and collected.

*Method B:* Crystalline $Ca[N(DIPP)(Si^iPr_3)]_2$ (63 mg, 0.089 mmol) was dissolved in benzene (0.8 mL) at room temperature, and $PhSiH_3$ (17.6 µL, 15.4 mg, 0.143 mmol, 1.6 eq.) and PMDTA (18.6 µL, 15.4 mg, 0.089 mmol, 1 eq.) were then consecutively added. This resulted in a clear pale yellow solution. Slow evaporation of the solvent from the reaction mixture overnight gave a uniform batch of small, colorless needle-like crystals of $Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (8 mg, 3.8 µmol) in 43% yield. These crystals were collected following decanting the remaining supernatant, washing with small amounts of cold pentane (−20 °C; 2 × 0.5 mL) and drying under reduced pressure at ambient temperature for 30 minutes.

*Method C:* $PhSiH_3$ (16.8 µL, 13.9 mg, 0.129 mmol, 1.5 eq.) was added at room temperature to an equimolar mixture of $Ca[N(DIPP)(Si^iPr_3)]_2$ (60 mg, 0.085 mmol) and PMDTA (17.7 µL, 14.7 mg, 0.085 mmol, 1 eq.) dissolved in toluene (0.8 mL). The resulting yellow solution was then stored at –20 °C for two weeks. Over this period, $Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (5 mg, 2.4 µL, 28%) crystallized in the form of pale yellow blocks, which were separated from the supernatant by decantation and collected after trituration with cold pentane (−20 °C; 2 × 0.5 mL) and removing residual volatile components in a dynamic vacuum at room temperature.

*Note:* Once crystallized, $Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ has a markedly negligible solubility in common organic deuterated solvents (such as $C_6D_6$, [$d_8$]PhMe, $C_6D_5Br$ or [$d_8$]THF), even at elevated temperatures, which precluded the acquisition of meaningful NMR spectroscopic data in solution. Attempts were made to obtain solution spectroscopic data on $Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ from the reaction mixture before it crystallized, but only complex product mixtures were observed. FT-IR (ATR, pure): $\tilde{\nu}$ = 2858 (w), 1406 (w), 1257 (w), 961 (w), 920 (m), 877 (w), 830 (w), 777 (w), 755 (m), 734 (m), 661 (m) $cm^{-1}$. Melting point: 220 – 224 °C (decomp.). Elemental analysis: calculated (%) for $C_{102}H_{214}Ca_{10}N_{10}Si_4$ (2094.02 $gmol^{-1}$; vacuum-dried sample): C 58.51, H 10.30, N 6.69; found: C 58.59, H 10.13, N 6.47.

**Synthesis of $Sr_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (2)**




This complex was prepared by two slightly different methods:

*Method A:* Crystalline $Sr[N(DIPP)(Si^iPr_3)]_2$ (99 mg, 0.131 mmol) was dissolved in toluene (0.7 mL), and $PhSiH_3$ (25.9 µL, 22.7 mg, 0.210 mmol, 1.6 eq.) and PMDTA (27.3 µL, 22.7 mg, 0.131 mmol, 1 eq.) were sequentially slowly added. The resultant clear pale yellow solution was then allowed to equilibrate with hexanes (3 mL reservoir) *via* vapor diffusion in a sealed vessel at ambient temperature over a period of the three days, during which time well-defined, colorless X-ray quality crystals of $Sr_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (12 mg, 4.7 µmol, 36%) separated. Following decanting the supernatant reaction solution, the crystals formed were washed multiple times with cold pentane (−20 °C; 3 × 1 mL), extensively vacuum-dried at room temperature for complete removal of toluene enclosed in the crystal lattice and collected.

*Method B:* A solution of $Sr[N(DIPP)(Si^iPr_3)]_2$ (97 mg, 0.129 mmol) in benzene (0.6 mL) was carefully treated with $PhSiH_3$ (25.6 µL, 22.5 mg, 0.207 mmol, 1.6 eq.), followed by the addition of PMDTA (27 µL, 22.4 mg, 0.129 mmol, 1 eq.). Upon slow evaporation of benzene from the resultant light yellow solution at room temperature in a glovebox overnight, well-defined, colorless needle-shaped crystals formed, which were isolated from the remaining supernatant by decantation and washed twice with cold pentane (−20 °C; 2 × 1 mL). Subsequent prolonged drying *in vacuo* at ambient temperature gave $Sr_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (14 mg, 5.4 µmol) as analytically pure crystalline solid in 42% yield.

*Note:* The markedly low solubility of $Sr_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ in common organic deuterated solvents once crystallized precluded attempts to characterize it by NMR spectroscopy in solution. FT-IR (ATR, pure): $\tilde{\nu}$ = 2940 (w), 2856 (m), 1457 (w), 1406 (m), 1332 (m), 1269 (m), 928 (s), 877 (s), 802 (w),

771 (s), 753 (s), 726 (s), 700 (s), 641 (s) $cm^{-1}$. Melting point: 216 – 219 °C (decomp.). Elemental analysis: calculated (%) for $C_{102}H_{214}N_{10}Si_4Sr_{10}$ (2569.44 $gmol^{-1}$; vacuum-dried sample): C 47.68, H 8.40, N 5.45; found: C 47.63, H 8.33, N 5.28.

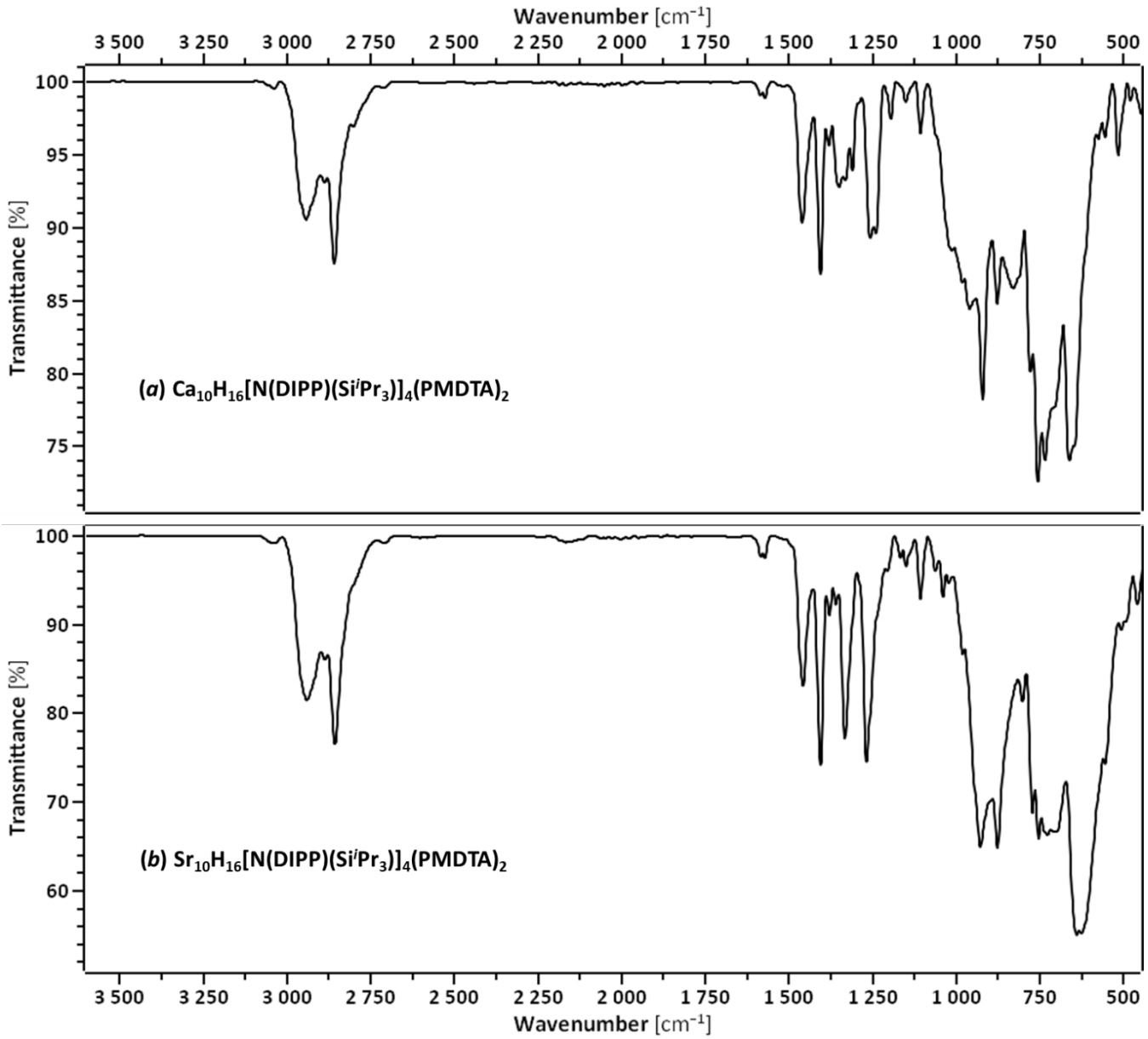



**Figure S1.** Stacked FT-IR ATR spectra of (*a*) $Ca_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4(PMDTA)_2$ (**1**) and (*b*) $Sr_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4(PMDTA)_2$ (**2**).

# 3 Crystal Structure Determination

**Structure determination of $Ca_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4(PMDTA)_2$ (1)**

A colorless crystal of compound $Ca_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4(PMDTA)_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(2) K in a $N_2$ gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas detector using a CuK$\alpha$ microfocus source. The measured data was processed with the CrysAlis$^{Pro}$ (v40.53) software package.[2] Using Olex2,[3] the structure was solved with the ShelXT[4] structure solution program using Intrinsic Phasing and refined with the ShelXL[5] refinement package using Least Squares minimization. All non-hydrogen atoms were refined anisotropically. Most hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The positions of the metal bound hydrides were observed from difference Fourier maps and refined.

Disorder of two $^{i}$Pr groups was observed and was modeled with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU).[6] The relative occupancies of the two alternative orientations were refined to 0.788(6)/0.212(6) and 0.56(2)/0.44(2), respectively.

Additionally, voids with heavily disordered solvent (mixture of toluene/*n*-hexane) were found within the crystal. A suitable disorder model for these solvent molecules could not be built. Therefore, their contribution to the structure factors was secured by back-Fourier transformation using the solvent mask routine[7,8] of the program Olex2.[3] The solvent accessible voids treated this way had a size of 8249.1 Å$^3$ (24.1% of the unit cell) and contained 1886.1 electrons/unit cell.

The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1970934 contains the supplementary crystallographic data for complex $Ca_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4(PMDTA)_2$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Crystallographic and refinement data are summarized in Table S1.

**Structure determination of $Sr_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (2)**

A colorless crystal of the composition $Sr_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2 \cdot (PhMe)_3$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then cooled to 240.0(1) K in a $N_2$ gas stream and kept at this temperature during the experiment. A low temperature measurement was not possible due to a phase transition, which reproducibly destroyed such crystals upon further cooling. The crystal structure was measured on a SuperNova diffractometer with Atlas detector using a CuK$\alpha$ microfocus source. The measured data was processed with the CrysAlis$^{Pro}$ (v40.53) software package.[2] Using Olex2,[3] the structure was solved with the ShelXT[4] structure solution program using Intrinsic Phasing and refined with the ShelXL[5] refinement package using Least Squares minimization. All non-hydrogen atoms were refined anisotropically. Most hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The positions of the metal bound hydrides were observed from difference Fourier maps and refined.

Disorder of six $^i$Pr groups and one PMDTA ligand was observed and was modeled with the help of similarity restraints (SIMU, SADI). The relative occupancies of the two alternative orientations were refined to 0.544(6)/0.456(6) (3 × $^i$Pr), 0.638(7)/0.362(7) (3 × $^i$Pr) and 0.715(9)/0.285(9) (PMDTA), respectively.

The three symmetry-independent toluene molecules within the unit cell were also heavily disordered. For two of them, it was possible to build a decent disorder model with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU).[6] It was also necessary to refine the aromatic rings as rigid hexagons (AFIX 66) and to apply a FLAT restrain to keep the methyl group of toluene in the plane of the aromatic ring. The relative occupancies of the two alternative orientations of these toluene molecules were refined to 0.795(12)/0.205(12) and 0.629(11)/0.371(1), respectively.

The contribution of the third toluene to the structure factors was secured by back-Fourier transformation using the solvent mask routine[7,8] of the program Olex2.[3] The voids treated this way had a size of 608.5 Å$^3$ (8.1% of the unit cell) and contained 106.9 electrons/unit cell.

The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1970936 contains the supplementary crystallographic data for complex

$Sr_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2\cdot(PhMe)_3$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

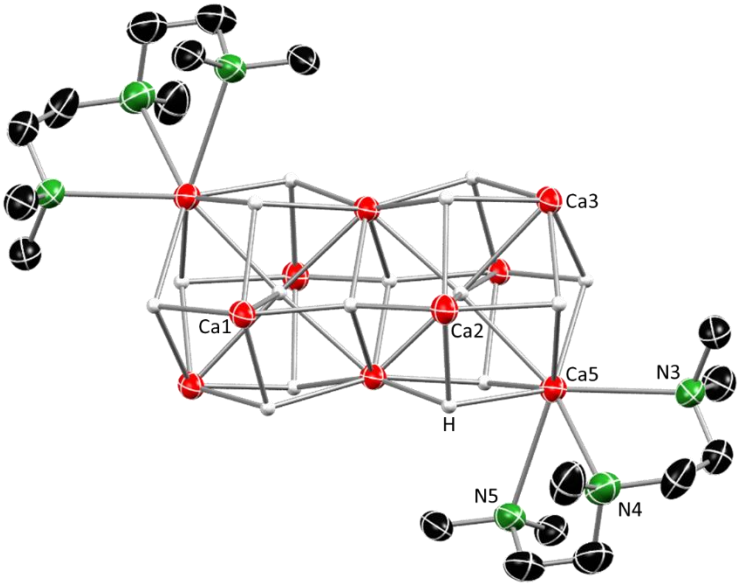
Crystallographic and refinement data are summarized in Table S1.

**Table S1.** Crystallographic data and structure refinement for $Ae_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (Ae = Ca, Sr).

| **Compound** | **$Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$ (1)** | **$Sr_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2 \cdot (PhMe)_3$ (2)** |
|---|---|---|
| **Empirical formula** | $C_{102}H_{214}Ca_{10}N_{10}Si_4$[a] | $C_{123}H_{238}Sr_{10}N_{10}Si_4$ |
| **Formula weight** [gmol$^{-1}$] | 2093.98[a] | 2845.78 |
| **Temperature** [K] | 100.0(2) | 240.0(1) |
| **Crystal system** | trigonal | triclinic |
| **Space group** | $R\bar{3}$ | $P\bar{1}$ |
| $\boldsymbol{a}$ [Å] | 46.5535(3) | 15.0995(3) |
| $\boldsymbol{b}$ [Å] | 46.5535(3) | 18.8526(3) |
| $\boldsymbol{c}$ [Å] | 18.2299(2) | 28.8886(5) |
| $\boldsymbol{\alpha}$ [°] | 90 | 100.4131(14) |
| $\boldsymbol{\beta}$ [°] | 90 | 91.1677(13) |
| $\boldsymbol{\gamma}$ [°] | 120 | 110.9442(15) |
| **Volume** [Å$^3$] | 34215.2(6) | 7521.3(2) |
| **Z** | 9 | 2 |
| $\boldsymbol{\rho_{Cald}}$ [gcm$^{-3}$] | 0.915[a] | 1.257 |
| $\boldsymbol{\mu}$ [mm$^{-1}$] | 3.575[a] | 5.048 |
| **F(000)** | 10368.0[a] | 2964.0 |
| **Crystal size** [mm$^3$] | 0.343 × 0.227 × 0.185 | 0.243 × 0.124 × 0.06 |
| **Radiation** | CuK$\alpha$ ($\lambda$ = 1.54184) | CuK$\alpha$ ($\lambda$ = 1.54184) |
| **2Θ range for data collection** [°] | 7.562 to 145.584 | 7.24 to 146.162 |
| **Index ranges** | -56 ≤ h ≤ 55<br>-55 ≤ k ≤ 57<br>-22 ≤ l ≤ 22 | -18 ≤ h ≤ 16<br>-23 ≤ k ≤ 23<br>-35 ≤ l ≤ 35 |
| **Reflections collected** | 70540 | 101674 |
| **Independent reflections** | 14967 | 29119 |
| **$R_{int}$** | 0.0318 | 0.0470 |
| **Data / restraints / parameters** | 14967 / 147 / 675 | 29119 / 3528 / 1729 |
| **Goodness-of-fit on F$^2$** | 1.056 | 1.035 |
| **Final R indexes** [$I \geq 2\sigma\ (I)$] | $R_1$ = 0.0442<br>$wR_2$ = 0.1152 | $R1$ = 0.0591<br>$wR_2$ = 0.1555 |
| **Final R indexes** [all data] | $R_1$ = 0.0491<br>$wR_2$ = 0.1210 | $R1$ = 0.0692<br>$wR_2$ = 0.1639 |
| **Largest diff. peak / hole** [eÅ$^{-3}$] | 0.82 / -0.28 | 1.86 / -0.78 |
| **CCDC number** | 1970934 | 1970936 |

[a] Contribution of the masked disordered solvent neglected.

(*a*)




(*b*)

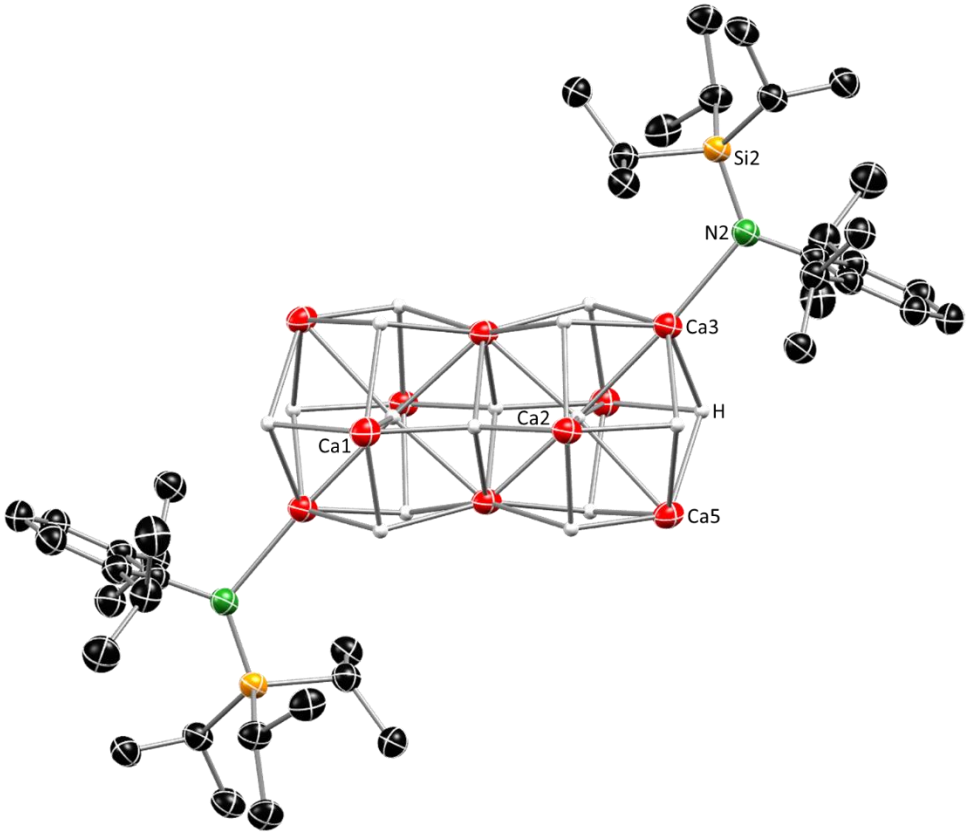



**Figure S2.** ORTEP representation of the centrosymmetric $Ca_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4(PMDTA)_2$ cluster showing the $Ca_{10}H_{16}^{4+}$ core of the complex and (*a*) the PMDTA and (*b*) the terminal *N*-bound ($^{i}Pr_3Si$)(DIPP)$N^-$ ligands, respectively. Thermal ellipsoids are displayed at 50% probability. Hydrogen atoms, except for the hydrides, have been omitted for clarity.

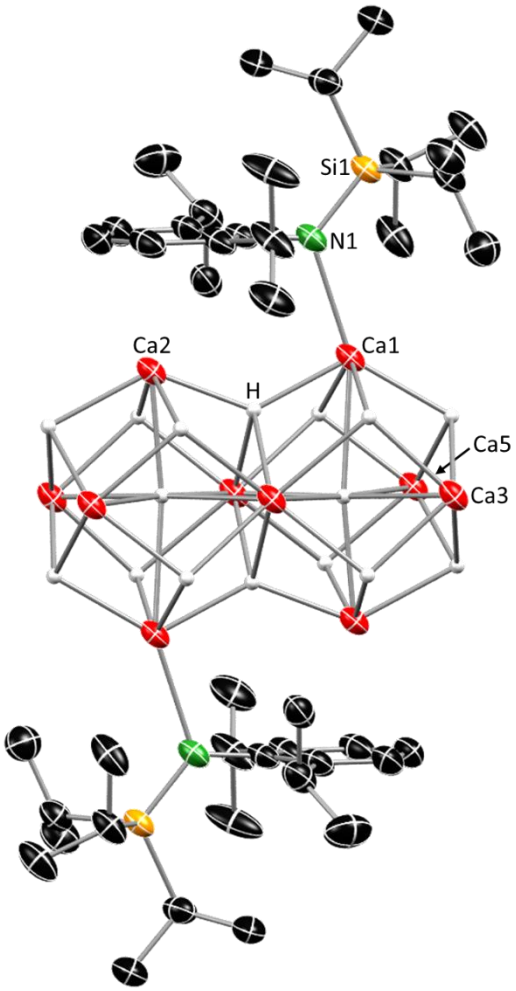
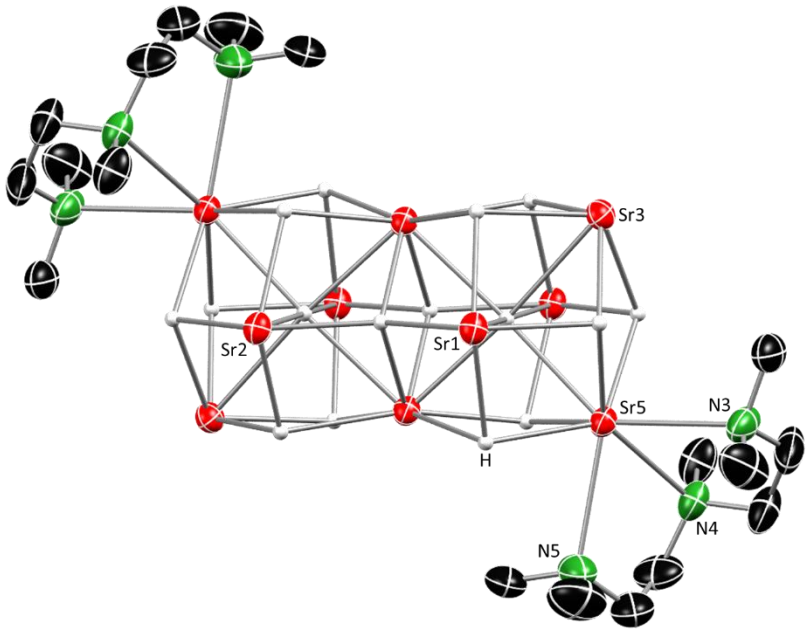



**Figure S3.** ORTEP representation of the centrosymmetric $Ca_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4(PMDTA)_2$ cluster showing the $Ca_{10}H_{16}^{4+}$ core of the complex and the (*N*,aryl)-bridging ($^{i}Pr_3Si$)(DIPP)$N^-$ ligands. Thermal ellipsoids are displayed at 50% probability. Hydrogen atoms of the ligands, as well as the disorder of the *iso*propyl groups, have been omitted for clarity.

(*a*)




(*b*)

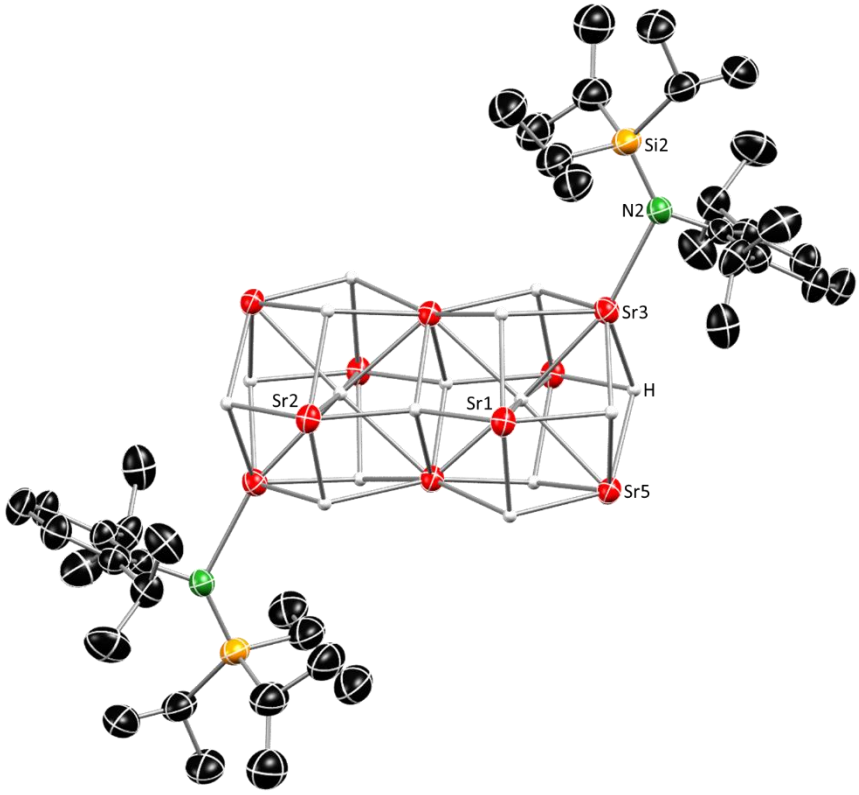



**Figure S4.** ORTEP representation of the centrosymmetric $Sr_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4(PMDTA)_2$ cluster showing the $Sr_{10}H_{16}^{4+}$ core of the complex and (*a*) the PMDTA and (*b*) the terminal *N*-bound ($^{i}Pr_3Si$)(DIPP)$N^-$ ligands, respectively. Thermal ellipsoids are displayed at 30% probability. Hydrogen atoms of the ligands, as well as the disorder, have been omitted for clarity.

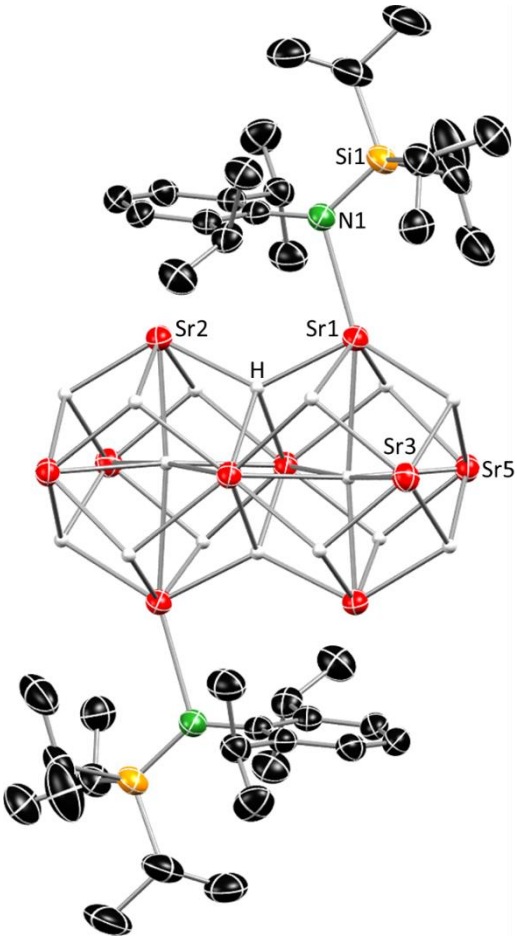


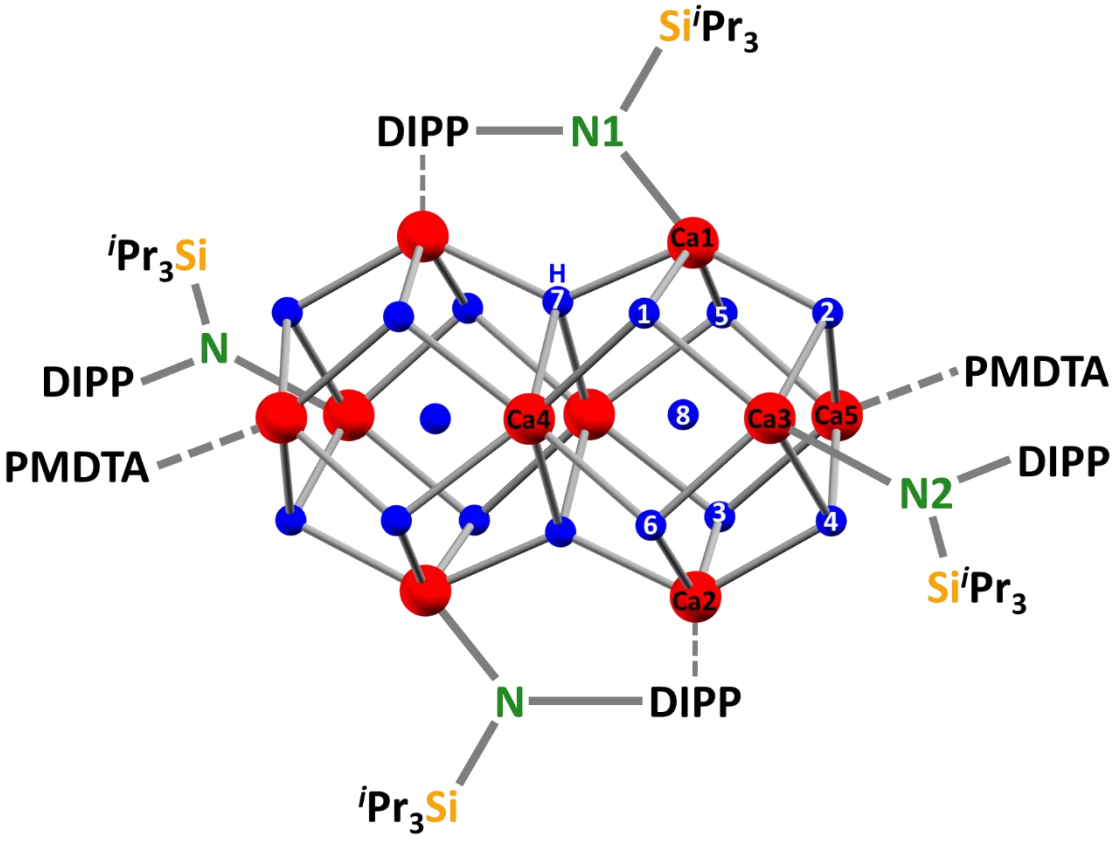

**Figure S5.** ORTEP representation of the centrosymmetric $Sr_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4(PMDTA)_2$ cluster showing the $Sr_{10}H_{16}^{4+}$ core and the (*N*,aryl)-bridging ($^{i}Pr_3Si$)(DIPP)$N^-$ ligands. Displacement ellipsoids are shown at the 30% probability level. Hydrogen atoms of the ligands, toluene solvate molecules in the lattice and the second symmetry-independent molecule, as well as the disorder, have been omitted for clarity.

# 4 Theoretical Calculations

### General Methods

All geometry optimizations were carried out using Gaussian 16A.[9] All methods were used as implemented. All structures were fully optimized on a B3PW91/def2TZVP level of theory.[10] In all cases Grimmeʿs third dispersion correction with Becke-Johnson damping (GD3BJ) was added.[11] Charges were calculated *via* NBO analyses.[12] Molecules were drawn and evaluated using Molecules (v2.311).[13]

**Table S2.** Comparison of selected experimental bond distances and calculated values (B3PW91/def2tzvp GB3DJ) for $Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4 \cdot (PMDTA)_2$.[a]




| | **Distances** [Å] | **Calculated distances** [Å] |
|---|---|---|
| **Ca···Ca** | | |
| Ca···Ca (*edge shared*) | 3.255(1) | 3.2415 |
| Ca···Ca (*other*) | 3.4348(8) – 3.6665(7)<br>**[3.5601]** | 3.3753 – 3.5657<br>**[3.4855]** |
| **$Ca–H_{center}$** | 2.41(2) – 2.67(5)<br>**[2.50]** | 2.39 – 2.54<br>**[2.45]** |
| **$Ca–H_{outer}$** | | |
| Ca–($\mu_4$-H) | 2.15(2) – 2.32(2)<br>**[2.24]** | 2.11 – 2.29<br>**[2.20]** |
| Ca–($\mu_3$-H) | 2.22(2) – 2.44(3)<br>**[2.32]** | 2.18 – 2.37<br>**[2.28]** |

**Table S2 (contd.).**

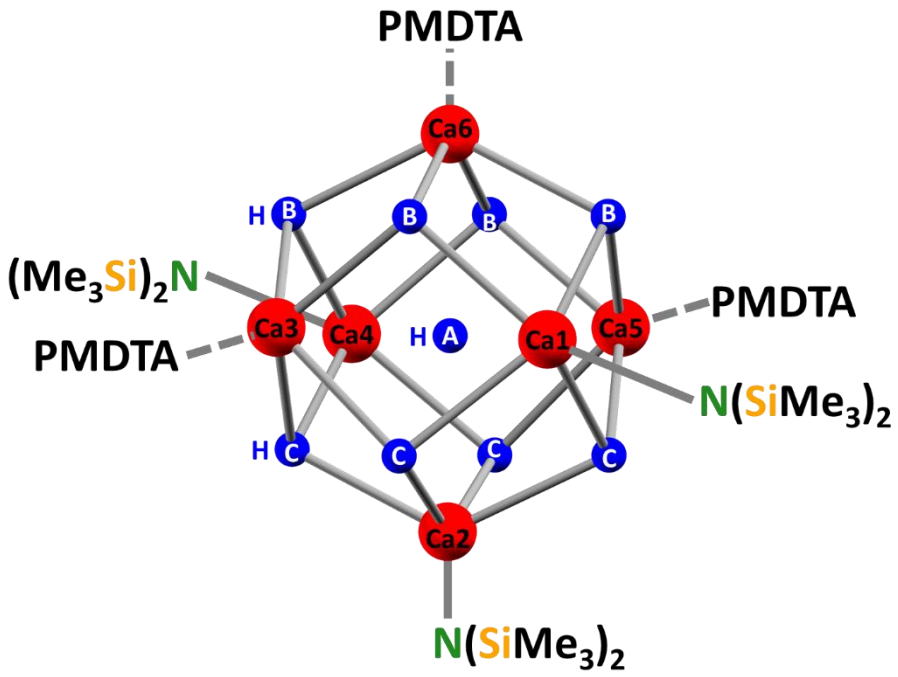
| | **Distances** [Å] | **Calculated distances** [Å] |
|---|---|---|
| **$H_{center}\cdots H_{center}$** | 3.58(4) | 3.58 |
| **$H_{center}\cdots H_{outer}$** | | |
| $H_{center}\cdots(\mu_4\text{-H})$ | 2.44(3) and 2.44(3) | 2.39 and 2.41 |
| $H_{center}\cdots(\mu_3\text{-H})$ | 2.44(3) – 2.62(4)<br>**[2.53]** | 2.45 – 2.58<br>**[2.49]** |
| **$H_{outer}\cdots H_{outer}$** | | |
| $(\mu_4\text{-H})\cdots(\mu_4\text{-H})$ | 3.32(4) | 3.20 |
| $(\mu_3\text{-H})\cdots(\mu_4\text{-H})$ | 2.67(3) – 2.79(3)<br>**[2.71]** | 2.67 – 2.73<br>**[2.69]** |
| $(\mu_3\text{-H})\cdots(\mu_3\text{-H})$ | 2.88(3) – 3.04(4)<br>**[2.93]** | 2.83 – 2.95<br>**[2.89]** |

[a] Average values shown in bold between square brackets.

**Table S3.** NPA charge analysis for $Ca_{10}H_{16}[N(DIPP)(Si^{i}Pr_3)]_4 \cdot (PMDTA)_2$ calculated at the B3PW91/def2tzvp GB3DJ level.

| Atom / Part | NPA charge |
|---|---|
| Ca1 | +1.69 |
| Ca2 | +1.66 |
| Ca3 | +1.70 |
| Ca4 | +1.67 |
| Ca5 | +1.67 |
| $\mu_3$-H1 | –0.83 |
| $\mu_3$-H2 | –0.83 |
| $\mu_3$-H3 | –0.83 |
| $\mu_3$-H4 | –0.82 |
| $\mu_3$-H5 | –0.83 |
| $\mu_3$-H6 | –0.82 |
| $\mu_4$-H7 | –0.83 |
| $H_{center}$ | –0.88 |
| N1 | –1.36 |
| N2 | –1.41 |
| Bridging ($^{i}Pr_3Si$)(DIPP)N | –0.90 |
| Terminal ($^{i}Pr_3Si$)(DIPP)N | –0.91 |
| PMDTA | +0.09 |

**Table S4.** Comparison of selected experimental bond distances and calculated values (B3PW91/def2tzvp GB3DJ) for $Ca_6H_9[N(SiMe_3)_2]_3 \cdot (PMDTA)_3$.[a]




| | Distances [Å][b] | Calculated distances [Å] |
|---|---|---|
| **Ca···Ca** | 3.4233(8) – 3.6058(9)<br>**[3.5113]** | 3.3720 – 3.5111<br>**[3.4368]** |
| **Ca–$H_{center}$** | 2.44(3) – 2.61(3)<br>**[2.48]** | 2.38 – 2.48<br>**[2.43]** |
| **Ca–$H_{outer}$** | 2.17(3) – 2.40(3)<br>**[2.30]** | 2.22 – 2.32<br>**[2.27]** |
| **$H_{center}$···$H_{outer}$** | 2.43(5) – 2.62(6)<br>**[2.53]** | 2.44 – 2.54<br>**[2.50]** |
| **$H_{outer}$···$H_{outer}$** | 2.78(4) – 3.05(5)<br>**[2.92]** | 2.75 – 2.98<br>**[2.89]** |

[a] Average values shown in bold between square brackets. [b] Data taken from Ref. 14 (CCDC number: 1559998).

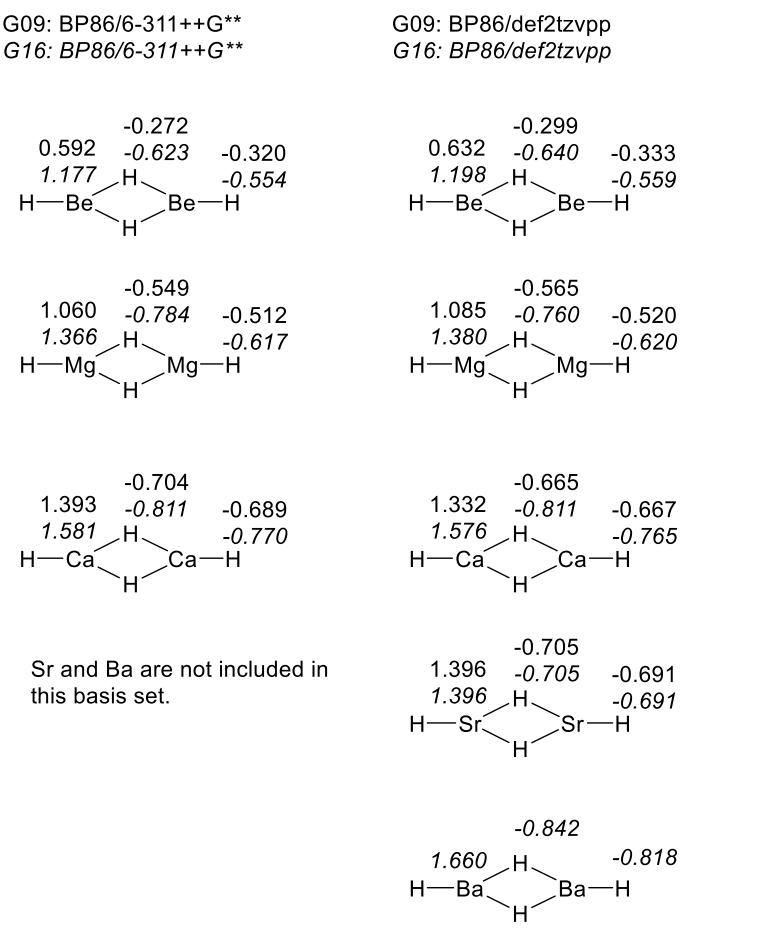
**Table S5.** NPA charge analysis for $Ca_6H_9[N(SiMe_3)_2]_3 \cdot (PMDTA)_3$ calculated at the B3PW91/def2tzvp GB3DJ level.

| Atom / Part | NPA charge |
|---|---|
| Ca1 | +1.66 |
| Ca2 | +1.70 |
| Ca3 | +1.69 |
| Ca4 | +1.69 |
| Ca5 | +1.66 |
| Ca6 | +1.66 |
| $H_{center}$ | –0.89 |
| $H_{outer}$ | −0.82 and –0.83 |
| $(Me_3Si)_2N$ | –0.93 |
| PMDTA | 0.07 – 0.08 |

**Discrepancies between NBO analysis in Gaussian09 and Gaussian16**

Although both, Gaussian09 and Gaussian16, incorporate NBO analysis with the NBO version 3.1, different values for atomic NPA charges on main group 2 metal species became apparent (see Figure S6). The reason for this difference, which is noticeable for Be, Mg and Ca complexes, is likely due to a difference in the assignment of valence and Rydberg orbitals. Guassian09 assigns *s*- and *p*- valence orbitals while in Gaussian16 only *s*-orbitals are used. NPA charges calculated with Gaussian16 are compatible to those calculated with older Gaussian versions (e.g. Gaussian03).

**Figure S6.** Calculation of NPA charges in group 2 metal hydride dimers with the NBO 3.1 program incorporated in Gaussian09 and Gaussian16 (numbers in italic) with different methods and basis sets.



## XYZ-Coordinates for Optimized Structures

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**$Ca_{10}H_{16}[N(DIPP)(Si^iPr_3)]_4(PMDTA)_2$**

| | | | |
|---|---|---|---|
| Ca | -1.834797 | -0.096363 | -2.584159 |
| Ca | 1.834797 | 0.096363 | 2.584159 |
| H | -1.647989 | -2.054840 | -1.480182 |
| H | 1.647989 | 2.054840 | 1.480182 |
| H | -3.839431 | -0.123082 | -1.613796 |
| H | 3.839431 | 0.123082 | 1.613796 |
| H | -1.825995 | 1.886296 | -1.569104 |
| H | 1.825995 | -1.886296 | 1.569104 |
| H | 0.052908 | -0.004342 | -1.598876 |
| H | -0.052908 | 0.004342 | 1.598876 |
| H | 1.787104 | 0.035175 | 0.047470 |
| H | -1.787104 | -0.035175 | -0.047470 |
| Ca | 2.029183 | 0.060749 | -2.333178 |
| Ca | -2.029183 | -0.060749 | 2.333178 |
| H | 1.884402 | -1.963145 | -1.378421 |
| H | -1.884402 | 1.963145 | 1.378421 |
| H | 3.938799 | 0.055966 | -1.272721 |
| H | -3.938799 | -0.055966 | 1.272721 |
| H | 1.804952 | 2.068311 | -1.349021 |
| H | -1.804952 | -2.068311 | 1.349021 |
| Ca | 3.478194 | 1.831548 | 0.148236 |
| Ca | -3.478194 | -1.831548 | -0.148236 |
| Ca | -0.050727 | 1.619854 | -0.017924 |
| Ca | 0.050727 | -1.619854 | 0.017924 |
| Ca | -3.558093 | 1.688493 | -0.154670 |
| Ca | 3.558093 | -1.688493 | 0.154670 |
| Si | -2.059377 | 0.255118 | -6.054995 |
| Si | 2.059377 | -0.255118 | 6.054995 |

| | | | |
|---|---|---|---|
| Si | 4.595121 | 5.019593 | -0.132276 |
| Si | -4.595121 | -5.019593 | 0.132276 |
| N | -0.929818 | 0.127083 | -4.786259 |
| N | 0.929818 | -0.127083 | 4.786259 |
| N | 5.168205 | 3.412882 | -0.025365 |
| N | -5.168205 | -3.412882 | 0.025365 |
| N | -6.168164 | 1.692456 | -0.733514 |
| N | 6.168164 | -1.692456 | 0.733514 |
| N | -4.984505 | 3.191059 | 1.513171 |
| N | 4.984505 | -3.191059 | -1.513171 |
| N | -2.828875 | 4.249190 | -0.286871 |
| N | 2.828875 | -4.249190 | 0.286871 |
| C | 0.430627 | 0.118609 | -4.858097 |
| C | -0.430627 | -0.118609 | 4.858097 |
| C | 1.190898 | 1.332541 | -4.878241 |
| C | -1.190898 | -1.332541 | 4.878241 |
| C | 2.581128 | 1.299568 | -4.831132 |
| C | -2.581128 | -1.299568 | 4.831132 |
| H | 3.133118 | 2.231500 | -4.813089 |
| H | -3.133118 | -2.231500 | 4.813089 |
| C | 3.280314 | 0.097080 | -4.830284 |
| C | -3.280314 | -0.097080 | 4.830284 |
| H | 4.360587 | 0.086843 | -4.808485 |
| H | -4.360587 | -0.086843 | 4.808485 |
| C | 2.559619 | -1.087188 | -4.915382 |
| C | -2.559619 | 1.087188 | 4.915382 |
| H | 3.094873 | -2.024084 | -4.995940 |
| H | -3.094873 | 2.024084 | 4.995940 |
| C | 1.170225 | -1.106580 | -4.930477 |
| C | -1.170225 | 1.106580 | 4.930477 |
| C | 0.449697 | -2.418296 | -5.122318 |
| C | -0.449697 | 2.418296 | 5.122318 |

| | | | |
|---|---|---|---|
| H | -0.539269 | -2.155643 | -5.500690 |
| H | 0.539269 | 2.155643 | 5.500690 |
| C | 1.128861 | -3.318472 | -6.151235 |
| C | -1.128861 | 3.318472 | 6.151235 |
| H | 1.350351 | -2.783447 | -7.075154 |
| H | -1.350351 | 2.783447 | 7.075154 |
| H | 0.476654 | -4.160731 | -6.392597 |
| H | -0.476654 | 4.160731 | 6.392597 |
| H | 2.064041 | -3.737065 | -5.769479 |
| H | -2.064041 | 3.737065 | 5.769479 |
| C | 0.264240 | -3.179810 | -3.815180 |
| C | -0.264240 | 3.179810 | 3.815180 |
| H | 1.230308 | -3.393944 | -3.352359 |
| H | -1.230308 | 3.393944 | 3.352359 |
| H | -0.249826 | -4.126835 | -3.995996 |
| H | 0.249826 | 4.126835 | 3.995996 |
| H | -0.319883 | -2.623224 | -3.078662 |
| H | 0.319883 | 2.623224 | 3.078662 |
| C | -2.294532 | 0.607426 | -8.878024 |
| C | 2.294532 | -0.607426 | 8.878024 |
| H | -2.774580 | -0.359894 | -9.047241 |
| H | 2.774580 | 0.359894 | 9.047241 |
| H | -1.822946 | 0.899637 | -9.822210 |
| H | 1.822946 | -0.899637 | 9.822210 |
| H | -3.082592 | 1.332768 | -8.664667 |
| H | 3.082592 | -1.332768 | 8.664667 |
| C | -3.113935 | -1.345061 | -6.074327 |
| C | 3.113935 | 1.345061 | 6.074327 |
| H | -2.552258 | -2.031766 | -6.723468 |
| H | 2.552258 | 2.031766 | 6.723468 |
| C | -4.513167 | -1.191909 | -6.668161 |
| C | 4.513167 | 1.191909 | 6.668161 |

| | | | |
|---|---|---|---|
| H | -5.147389 | -0.576842 | -6.024607 |
| H | 5.147389 | 0.576842 | 6.024607 |
| H | -5.007776 | -2.163910 | -6.768576 |
| H | 5.007776 | 2.163910 | 6.768576 |
| H | -4.500580 | -0.725926 | -7.654431 |
| H | 4.500580 | 0.725926 | 7.654431 |
| C | -3.203788 | -2.006231 | -4.700951 |
| C | 3.203788 | 2.006231 | 4.700951 |
| H | -2.221826 | -2.226413 | -4.281841 |
| H | 2.221826 | 2.226413 | 4.281841 |
| H | -3.746885 | -2.954598 | -4.743054 |
| H | 3.746885 | 2.954598 | 4.743054 |
| H | -3.760743 | -1.387019 | -3.987627 |
| H | 3.760743 | 1.387019 | 3.987627 |
| C | -3.294206 | 1.688294 | -5.798863 |
| C | 3.294206 | -1.688294 | 5.798863 |
| H | -4.157899 | 1.406925 | -6.412466 |
| H | 4.157899 | -1.406925 | 6.412466 |
| C | -3.758534 | 1.744380 | -4.350977 |
| C | 3.758534 | -1.744380 | 4.350977 |
| H | -4.161564 | 0.791627 | -3.994932 |
| H | 4.161564 | -0.791627 | 3.994932 |
| H | -4.547821 | 2.488636 | -4.208110 |
| H | 4.547821 | -2.488636 | 4.208110 |
| H | -2.936034 | 2.042182 | -3.688455 |
| H | 2.936034 | -2.042182 | 3.688455 |
| C | -2.857955 | 3.080599 | -6.248556 |
| C | 2.857955 | -3.080599 | 6.248556 |
| H | -2.103451 | 3.496329 | -5.578675 |
| H | 2.103451 | -3.496329 | 5.578675 |
| H | -3.707347 | 3.773023 | -6.237959 |
| H | 3.707347 | -3.773023 | 6.237959 |

| | | | |
|---|---|---|---|
| H | -2.443020 | 3.088367 | -7.257870 |
| H | 2.443020 | -3.088367 | 7.257870 |
| C | 6.503802 | 3.024740 | -0.053968 |
| C | -6.503802 | -3.024740 | 0.053968 |
| C | 7.155199 | 2.676873 | -1.269073 |
| C | -7.155199 | -2.676873 | 1.269073 |
| C | 8.475551 | 2.243794 | -1.266894 |
| C | -8.475551 | -2.243794 | 1.266894 |
| H | 8.946634 | 1.990382 | -2.211544 |
| H | -8.946634 | -1.990382 | 2.211544 |
| C | 9.205904 | 2.137668 | -0.096081 |
| C | -9.205904 | -2.137668 | 0.096081 |
| H | 10.238429 | 1.808827 | -0.112260 |
| H | -10.238429 | -1.808827 | 0.112260 |
| C | 8.583864 | 2.465320 | 1.096492 |
| C | -8.583864 | -2.465320 | -1.096492 |
| H | 9.140466 | 2.380175 | 2.024096 |
| H | -9.140466 | -2.380175 | -2.024096 |
| C | 7.264122 | 2.897303 | 1.142217 |
| C | -7.264122 | -2.897303 | -1.142217 |
| C | 6.439222 | 2.786048 | -2.592967 |
| C | -6.439222 | -2.786048 | 2.592967 |
| H | 5.445155 | 3.171863 | -2.371700 |
| H | -5.445155 | -3.171863 | 2.371700 |
| C | 7.140540 | 3.764261 | -3.533591 |
| C | -7.140540 | -3.764261 | 3.533591 |
| H | 7.324659 | 4.721430 | -3.042810 |
| H | -7.324659 | -4.721430 | 3.042810 |
| H | 6.535933 | 3.946562 | -4.426473 |
| H | -6.535933 | -3.946562 | 4.426473 |
| H | 8.107990 | 3.373796 | -3.860718 |
| H | -8.107990 | -3.373796 | 3.860718 |

| | | | |
|---|---|---|---|
| C | 6.267483 | 1.427534 | -3.266179 |
| C | -6.267483 | -1.427534 | 3.266179 |
| H | 7.228948 | 0.921949 | -3.392117 |
| H | -7.228948 | -0.921949 | 3.392117 |
| H | 5.827155 | 1.551803 | -4.258974 |
| H | -5.827155 | -1.551803 | 4.258974 |
| H | 5.608404 | 0.783583 | -2.677883 |
| H | -5.608404 | -0.783583 | 2.677883 |
| C | 6.657205 | 3.187219 | 2.495216 |
| C | -6.657205 | -3.187219 | -2.495216 |
| H | 5.685544 | 3.644848 | 2.308909 |
| H | -5.685544 | -3.644848 | -2.308909 |
| C | 6.424470 | 1.894243 | 3.273780 |
| C | -6.424470 | -1.894243 | -3.273780 |
| H | 5.678423 | 1.266113 | 2.780278 |
| H | -5.678423 | -1.266113 | -2.780278 |
| H | 6.069678 | 2.104250 | 4.283894 |
| H | -6.069678 | -2.104250 | -4.283894 |
| H | 7.350589 | 1.318972 | 3.354163 |
| H | -7.350589 | -1.318972 | -3.354163 |
| C | 7.497231 | 4.156405 | 3.323923 |
| C | -7.497231 | -4.156405 | -3.323923 |
| H | 8.438931 | 3.700566 | 3.640392 |
| H | -8.438931 | -3.700566 | -3.640392 |
| H | 6.957911 | 4.453306 | 4.227462 |
| H | -6.957911 | -4.453306 | -4.227462 |
| H | 7.741346 | 5.056471 | 2.757987 |
| H | -7.741346 | -5.056471 | -2.757987 |
| C | 2.872574 | 4.967741 | 0.691321 |
| C | -2.872574 | -4.967741 | -0.691321 |
| H | 2.344572 | 4.107297 | 0.244260 |
| H | -2.344572 | -4.107297 | -0.244260 |

| | | | |
|---|---|---|---|
| C | 2.998323 | 4.700117 | 2.188166 |
| C | -2.998323 | -4.700117 | -2.188166 |
| H | 3.589422 | 3.807323 | 2.398269 |
| H | -3.589422 | -3.807323 | -2.398269 |
| H | 2.019212 | 4.550315 | 2.648216 |
| H | -2.019212 | -4.550315 | -2.648216 |
| H | 3.488036 | 5.534826 | 2.696840 |
| H | -3.488036 | -5.534826 | -2.696840 |
| C | 1.963360 | 6.167974 | 0.438329 |
| C | -1.963360 | -6.167974 | -0.438329 |
| H | 2.419413 | 7.101609 | 0.772148 |
| H | -2.419413 | -7.101609 | -0.772148 |
| H | 1.019434 | 6.058189 | 0.984455 |
| H | -1.019434 | -6.058189 | -0.984455 |
| H | 1.722537 | 6.282017 | -0.619189 |
| H | -1.722537 | -6.282017 | 0.619189 |
| C | 4.403175 | 5.598841 | -1.940035 |
| C | -4.403175 | -5.598841 | 1.940035 |
| H | 5.369007 | 5.339525 | -2.385793 |
| H | -5.369007 | -5.339525 | 2.385793 |
| C | 3.332949 | 4.792753 | -2.668184 |
| C | -3.332949 | -4.792753 | 2.668184 |
| H | 3.414562 | 3.717874 | -2.487488 |
| H | -3.414562 | -3.717874 | 2.487488 |
| H | 3.380870 | 4.955535 | -3.750524 |
| H | -3.380870 | -4.955535 | 3.750524 |
| H | 2.330776 | 5.085486 | -2.346103 |
| H | -2.330776 | -5.085486 | 2.346103 |
| C | 4.194308 | 7.092570 | -2.180997 |
| C | -4.194308 | -7.092570 | 2.180997 |
| H | 3.284442 | 7.464264 | -1.704816 |
| H | -3.284442 | -7.464264 | 1.704816 |

| | | | |
|---|---|---|---|
| H | 4.104674 | 7.302215 | -3.253451 |
| H | -4.104674 | -7.302215 | 3.253451 |
| H | 5.026553 | 7.687762 | -1.804042 |
| H | -5.026553 | -7.687762 | 1.804042 |
| C | 5.752374 | 6.218451 | 0.783556 |
| C | -5.752374 | -6.218451 | -0.783556 |
| H | 5.978975 | 5.687321 | 1.713420 |
| H | -5.978975 | -5.687321 | -1.713420 |
| C | 5.179120 | 7.576858 | 1.180713 |
| C | -5.179120 | -7.576858 | -1.180713 |
| H | 4.858959 | 8.161002 | 0.316031 |
| H | -4.858959 | -8.161002 | -0.316031 |
| H | 5.932288 | 8.171753 | 1.710303 |
| H | -5.932288 | -8.171753 | -1.710303 |
| H | 4.318921 | 7.479096 | 1.845704 |
| H | -4.318921 | -7.479096 | -1.845704 |
| C | 7.070848 | 6.380415 | 0.024006 |
| C | -7.070848 | -6.380415 | -0.024006 |
| H | 7.531870 | 5.417920 | -0.204343 |
| H | -7.531870 | -5.417920 | 0.204343 |
| H | 7.791655 | 6.961765 | 0.610178 |
| H | -7.791655 | -6.961765 | -0.610178 |
| H | 6.924693 | 6.910728 | -0.920872 |
| H | -6.924693 | -6.910728 | 0.920872 |
| C | -6.489321 | 1.785288 | -2.150409 |
| C | 6.489321 | -1.785288 | 2.150409 |
| H | -6.197862 | 2.763126 | -2.538157 |
| H | 6.197862 | -2.763126 | 2.538157 |
| H | -7.564658 | 1.643616 | -2.334822 |
| H | 7.564658 | -1.643616 | 2.334822 |
| H | -5.941631 | 1.016604 | -2.689475 |
| H | 5.941631 | -1.016604 | 2.689475 |

| | | | |
|---|---|---|---|
| C | -6.552841 | 0.364676 | -0.250668 |
| C | 6.552841 | -0.364676 | 0.250668 |
| H | -6.066001 | -0.385197 | -0.866209 |
| H | 6.066001 | 0.385197 | 0.866209 |
| H | -7.636227 | 0.203107 | -0.312533 |
| H | 7.636227 | -0.203107 | 0.312533 |
| H | -6.227387 | 0.210070 | 0.774188 |
| H | 6.227387 | -0.210070 | -0.774188 |
| C | -6.882319 | 2.728926 | 0.001651 |
| C | 6.882319 | -2.728926 | -0.001651 |
| H | -7.966194 | 2.531174 | 0.004189 |
| H | 7.966194 | -2.531174 | -0.004189 |
| H | -6.743428 | 3.675608 | -0.527514 |
| H | 6.743428 | -3.675608 | 0.527514 |
| C | -6.404230 | 2.849014 | 1.430455 |
| C | 6.404230 | -2.849014 | -1.430455 |
| H | -7.021346 | 3.587761 | 1.964867 |
| H | 7.021346 | -3.587761 | -1.964867 |
| H | -6.546478 | 1.896612 | 1.942113 |
| H | 6.546478 | -1.896612 | -1.942113 |
| C | -4.469462 | 2.852911 | 2.831823 |
| C | 4.469462 | -2.852911 | -2.831823 |
| H | -4.625117 | 1.788728 | 3.008421 |
| H | 4.625117 | -1.788728 | -3.008421 |
| H | -4.969616 | 3.425120 | 3.629040 |
| H | 4.969616 | -3.425120 | -3.629040 |
| H | -3.398086 | 3.036813 | 2.871195 |
| H | 3.398086 | -3.036813 | -2.871195 |
| C | -4.775543 | 4.607331 | 1.220903 |
| C | 4.775543 | -4.607331 | -1.220903 |
| H | -5.418715 | 4.888317 | 0.386869 |
| H | 5.418715 | -4.888317 | -0.386869 |

| | | | |
|---|---|---|---|
| H | -5.092022 | 5.226240 | 2.075579 |
| H | 5.092022 | -5.226240 | -2.075579 |
| C | -3.340362 | 4.946544 | 0.887642 |
| C | 3.340362 | -4.946544 | -0.887642 |
| H | -2.691624 | 4.675799 | 1.722841 |
| H | 2.691624 | -4.675799 | -1.722841 |
| H | -3.260966 | 6.039247 | 0.762743 |
| H | 3.260966 | -6.039247 | -0.762743 |
| C | -3.480748 | 4.652858 | -1.523765 |
| C | 3.480748 | -4.652858 | 1.523765 |
| H | -3.028372 | 4.103356 | -2.350143 |
| H | 3.028372 | -4.103356 | 2.350143 |
| H | -3.380290 | 5.731696 | -1.718949 |
| H | 3.380290 | -5.731696 | 1.718949 |
| H | -4.544582 | 4.409829 | -1.499119 |
| H | 4.544582 | -4.409829 | 1.499119 |
| C | -1.397110 | 4.493721 | -0.389211 |
| C | 1.397110 | -4.493721 | 0.389211 |
| H | -0.912533 | 4.164184 | 0.533975 |
| H | 0.912533 | -4.164184 | -0.533975 |
| H | -1.169126 | 5.561354 | -0.519125 |
| H | 1.169126 | -5.561354 | 0.519125 |
| H | -0.998624 | 3.951534 | -1.247389 |
| H | 0.998624 | -3.951534 | 1.247389 |
| C | 0.461785 | 2.639194 | -5.042397 |
| C | -0.461785 | -2.639194 | 5.042397 |
| H | -0.462330 | 2.374953 | -5.555449 |
| H | 0.462330 | -2.374953 | 5.555449 |
| C | 0.066351 | 3.266600 | -3.712309 |
| C | -0.066351 | -3.266600 | 3.712309 |
| H | 0.944399 | 3.464494 | -3.096700 |
| H | -0.944399 | -3.464494 | 3.096700 |

| | | | |
|---|---|---|---|
| H | -0.593426 | 2.607541 | -3.143625 |
| H | 0.593426 | -2.607541 | 3.143625 |
| H | -0.461950 | 4.210532 | -3.877719 |
| H | 0.461950 | -4.210532 | 3.877719 |
| C | 1.211141 | 3.634734 | -5.918486 |
| C | -1.211141 | -3.634734 | 5.918486 |
| H | 0.561960 | 4.481464 | -6.153052 |
| H | -0.561960 | -4.481464 | 6.153052 |
| H | 1.528565 | 3.178698 | -6.858715 |
| H | -1.528565 | -3.178698 | 6.858715 |
| H | 2.094869 | 4.036568 | -5.418880 |
| H | -2.094869 | -4.036568 | 5.418880 |
| C | -1.258621 | 0.511470 | -7.757725 |
| C | 1.258621 | -0.511470 | 7.757725 |
| H | -0.748479 | 1.481234 | -7.686870 |
| H | 0.748479 | -1.481234 | 7.686870 |
| C | -0.206542 | -0.537044 | -8.105396 |
| C | 0.206542 | 0.537044 | 8.105396 |
| H | 0.623721 | -0.529337 | -7.399796 |
| H | -0.623721 | 0.529337 | 7.399796 |
| H | 0.206441 | -0.360626 | -9.104730 |
| H | -0.206441 | 0.360626 | 9.104730 |
| H | -0.633845 | -1.543972 | -8.108788 |
| H | 0.633845 | 1.543972 | 8.108788 |

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**$Ca_6H_9[N(SiMe_3)_2]_3(PMDTA)_3$**

| | | | |
|---|---|---|---|
| Ca | -0.964424 | 0.502407 | 2.419786 |
| Ca | -1.264057 | 1.944660 | -0.653006 |
| Ca | -2.080790 | -1.393535 | -0.203701 |
| Ca | 1.855180 | 1.224255 | 0.630439 |
| Ca | 0.651891 | -0.489043 | -2.089182 |
| Ca | 0.991917 | -2.054005 | 1.018005 |
| Si | -2.045469 | 4.992141 | -1.597791 |
| Si | -4.353806 | 3.031114 | -1.852460 |
| Si | -2.951115 | -4.742113 | 0.645942 |
| Si | -4.859402 | -2.977494 | -0.869217 |
| Si | 5.120364 | 1.603520 | 1.462670 |
| Si | 3.675142 | 4.117786 | 0.572964 |
| N | -3.378703 | -3.308787 | -0.127119 |
| N | -2.777521 | 3.482950 | -1.445194 |
| N | -2.487145 | 2.455891 | 3.310930 |
| N | 3.773618 | 2.470275 | 0.952453 |
| N | 2.729503 | -3.984390 | 0.338771 |
| N | 2.913049 | 0.180581 | -3.276194 |
| N | 0.139511 | 0.737248 | -4.361177 |
| N | 1.837446 | -3.308149 | 3.165634 |
| N | -0.312185 | -2.204585 | -3.842159 |
| N | -3.080733 | -0.481997 | 3.667992 |
| N | 0.292995 | 1.836991 | 4.319776 |
| C | -5.215361 | 2.278653 | -0.349235 |
| H | -4.555406 | 1.552678 | 0.134289 |
| H | -6.157059 | 1.782114 | -0.595732 |
| H | -5.428454 | 3.071632 | 0.374293 |
| C | -4.318916 | 1.770016 | -3.256844 |
| H | -3.977238 | 2.264532 | -4.171305 |
| H | -5.293314 | 1.317972 | -3.458052 |

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|---|---|---|---|
| H | -3.611158 | 0.969502 | -3.025544 |
| C | 3.883511 | 0.640728 | -2.287063 |
| H | 3.482287 | 1.481748 | -1.723500 |
| H | 4.815977 | 0.972724 | -2.768209 |
| H | 4.106571 | -0.165937 | -1.592968 |
| C | -2.817186 | 6.348573 | -0.538835 |
| H | -3.843422 | 6.555051 | -0.851481 |
| H | -2.252926 | 7.283549 | -0.604729 |
| H | -2.845296 | 6.045140 | 0.511126 |
| C | -2.617229 | 3.456424 | 2.252526 |
| H | -1.638022 | 3.853692 | 1.992412 |
| H | -3.268231 | 4.286560 | 2.564178 |
| H | -3.046912 | 3.004484 | 1.359452 |
| C | -1.677075 | -2.561449 | -3.462266 |
| H | -1.670362 | -3.057503 | -2.490855 |
| H | -2.125349 | -3.246705 | -4.197152 |
| H | -2.294262 | -1.667978 | -3.387907 |
| C | 2.129853 | -5.169164 | -0.261077 |
| H | 1.420466 | -5.625805 | 0.424250 |
| H | 2.879596 | -5.923959 | -0.534195 |
| H | 1.578564 | -4.878139 | -1.154676 |
| C | -1.959222 | 5.649590 | -3.364118 |
| H | -1.473098 | 4.922984 | -4.020421 |
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| H | 4.188428 | 4.004201 | -1.848087 |
| H | 3.108676 | 5.374029 | -1.539179 |
| H | 2.465229 | 3.728820 | -1.565685 |
| C | 2.275464 | 4.915757 | 1.556723 |
| H | 1.358418 | 4.323937 | 1.482536 |
| H | 2.045190 | 5.928491 | 1.216626 |

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|---|---|---|---|
| H | 2.555900 | 4.967893 | 2.613037 |
| C | -5.162535 | -3.922933 | -2.471621 |
| H | -4.352339 | -3.748390 | -3.183734 |
| H | -6.098844 | -3.614175 | -2.945732 |
| H | -5.215757 | -4.999053 | -2.292211 |
| C | 3.512123 | -0.900684 | -4.047642 |
| H | 3.882411 | -1.674331 | -3.371875 |
| H | 4.365449 | -0.543846 | -4.646387 |
| H | 2.788154 | -1.346705 | -4.729687 |
| C | -1.872281 | 3.058978 | 4.493098 |
| H | -2.269852 | 4.071847 | 4.658201 |
| H | -2.149822 | 2.480358 | 5.374406 |
| C | -0.756649 | -0.129543 | -5.125091 |
| H | -0.877589 | 0.234430 | -6.157677 |
| H | -1.739098 | -0.069295 | -4.654326 |
| C | 1.712239 | 2.038574 | 4.042047 |
| H | 2.199185 | 1.074726 | 3.906533 |
| H | 2.206956 | 2.586086 | 4.858635 |
| H | 1.838577 | 2.618322 | 3.128732 |
| C | 4.754677 | -4.003744 | -1.215591 |
| H | 5.390332 | -4.428369 | -0.418259 |
| H | 4.406393 | -4.843135 | -1.821032 |
| C | 3.449476 | -4.315082 | 1.568378 |
| H | 4.135911 | -3.493930 | 1.786129 |
| H | 4.067388 | -5.215867 | 1.443769 |
| C | -4.858216 | -1.147109 | -1.326880 |
| H | -4.763302 | -0.491979 | -0.456023 |
| H | -5.789293 | -0.859401 | -1.819101 |
| H | -4.061182 | -0.878726 | -2.028672 |
| N | 5.508467 | -3.114085 | -2.081285 |
| C | 3.558932 | -3.263555 | -0.628903 |
| H | 3.890296 | -2.343191 | -0.151383 |

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| H | 2.909867 | -2.950805 | -1.448783 |
| C | -0.293193 | -1.572952 | -5.159824 |
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| H | 0.727663 | -1.628995 | -5.544479 |
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| H | -1.446599 | 1.815180 | -3.505768 |
| H | -0.794377 | 2.542270 | -4.986059 |
| H | 0.118718 | 2.633961 | -3.462770 |
| C | 6.548512 | 1.552554 | 0.229222 |
| H | 6.215459 | 1.166208 | -0.736719 |
| H | 7.368082 | 0.919852 | 0.583386 |
| H | 6.952148 | 2.553617 | 0.059341 |
| C | -5.478021 | 4.429980 | -2.437303 |
| H | -5.603071 | 5.192333 | -1.664559 |
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| H | -5.084279 | 4.919581 | -3.331209 |
| C | -6.363238 | -3.268958 | 0.229340 |
| H | -6.472917 | -4.330661 | 0.467079 |
| H | -7.287023 | -2.941094 | -0.255868 |
| H | -6.265597 | -2.727734 | 1.173803 |
| C | 2.533149 | 1.312545 | -4.123959 |
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| H | 2.243444 | 2.126692 | -3.456956 |
| C | 1.394206 | 0.996562 | -5.068960 |
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| H | 1.651264 | 0.128273 | -5.675531 |
| C | 2.512360 | -4.534593 | 2.743245 |
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| H | -4.297291 | 1.698927 | 2.660429 |

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| C | 0.694918 | -3.610485 | 4.019950 |
| H | 0.176299 | -2.683058 | 4.262193 |
| H | 1.006871 | -4.095179 | 4.957638 |
| H | -0.002914 | -4.265861 | 3.501836 |
| C | -0.259729 | 4.818376 | -1.009274 |
| H | -0.197328 | 4.496570 | 0.035115 |
| H | 0.277837 | 5.766757 | -1.070525 |
| H | 0.315605 | 4.100543 | -1.602823 |
| C | 4.591252 | -0.194615 | 1.732165 |
| H | 3.840111 | -0.245786 | 2.523947 |
| H | 5.434074 | -0.830031 | 2.017703 |
| H | 4.132395 | -0.611129 | 0.829581 |
| C | 5.842430 | 2.164230 | 3.112145 |
| H | 6.263673 | 3.169130 | 3.036186 |
| H | 6.637057 | 1.495257 | 3.456306 |
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| C | -0.364301 | 3.142533 | 4.392387 |
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| H | -0.083801 | 3.685196 | 3.488132 |
| C | 0.152744 | 1.072914 | 5.548400 |
| H | -0.895572 | 0.869210 | 5.767324 |
| H | 0.587410 | 1.594553 | 6.415546 |
| H | 0.666602 | 0.116530 | 5.434251 |
| C | -3.719552 | 0.601519 | 4.410861 |

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| H | -4.733868 | 0.313083 | 4.728967 |
| H | -3.148419 | 0.763060 | 5.328447 |
| C | 2.747596 | -2.433587 | 3.897373 |
| H | 3.635623 | -2.218728 | 3.308497 |
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| H | 2.250005 | -1.483395 | 4.089262 |
| C | 6.334909 | -2.183501 | -1.337961 |
| H | 5.741368 | -1.610453 | -0.627786 |
| H | 6.798571 | -1.473285 | -2.023954 |
| H | 7.137392 | -2.693061 | -0.776369 |
| C | -3.746834 | -4.966564 | 2.344209 |
| H | -3.468622 | -4.148442 | 3.013251 |
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| C | 5.219773 | 5.133581 | 0.947254 |
| H | 5.446887 | 5.136316 | 2.015962 |
| H | 5.074307 | 6.172546 | 0.636728 |
| H | 6.096025 | 4.750909 | 0.418237 |
| C | -1.090442 | -4.741349 | 0.963422 |
| H | -0.559260 | -4.559575 | 0.027990 |
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| H | -0.887718 | -3.911124 | 1.647121 |
| C | -3.337677 | -6.303703 | -0.338929 |
| H | -4.416233 | -6.434707 | -0.460991 |
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| C | -2.655422 | -1.552857 | 4.557757 |
| H | -2.152264 | -2.315170 | 3.962692 |
| H | -3.501924 | -2.016447 | 5.086455 |
| H | -1.955883 | -1.169470 | 5.303924 |
| C | 6.299087 | -3.839421 | -3.051985 |
| H | 7.078118 | -4.469672 | -2.588128 |

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| H | 5.653926 | -4.482407 | -3.653912 |
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| H | -1.540645 | 0.043384 | -1.874223 |
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| H | -0.130852 | -0.083388 | 0.206850 |
| H | 0.885515 | 1.638353 | -1.366954 |
| H | -0.072868 | -2.322036 | -0.911031 |
| H | -2.457356 | 0.636003 | 0.742973 |
| H | -0.051969 | 2.220274 | 1.265980 |
| H | -1.060488 | -1.704425 | 1.835303 |

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