Supplementary Information for

Pathway to a Molecular Calcium Methyl

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Synthetic Details

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General Considerations

All manipulations were carried out using standard Schlenk line and glovebox techniques under an inert atmosphere of argon. NMR experiments were conducted in J-Young tap NMR tubes prepared in a glovebox. NMR spectra were recorded on a Bruker BioSpin GmbH spectrometer operating at 400.13 MHz (^{1}H) and 100.62 MHz (^{13}C). Elemental analyses were performed at Elemental Microanalysis Ltd., Okehampton, Devon, UK. Solvents were dried by passage through a commercially available solvent purification system and stored under argon in ampoules over 4 Å molecular sieves. C_6D_6 and C_7D_8 were purchased from Merck, dried over potassium before distilling and storage over molecular sieves. $[(BDI)CaH]_2$ (BDI = HC{(Me)CN-2,6-*i*-$Pr_2C_6H_3$}$_2$) was synthesised according to literature procedure.[1] $ZnMe_2$ was purchased from Merck as a 1.0 M standard solution in heptane, transferred to a J-Young's ampoule and used without further purification.

Initial Attempt to Synthesise $[(BDI)CaMe]_2$

$ZnMe_2$ (1.0 M in heptane, 32.6 µl, 0.033 mmol) was added to a J. Young's NMR tube containing a C_7D_8 (*ca.* 0.6 cm^3) solution of $[(BDI)CaH]_2$ (30 mg, 0.033 mmol). Initially three distinct CH_3 containing species were observed in the corresponding ^{1}H NMR spectrum, alongside the formation of free DippNacNac-H (**Figure S1**). Repeating the reaction with 2 equivalents of $ZnMe_2$, led exclusively to the formation of [(BDI)ZnMe] after 16 hours (**Figure S2**), identified spectroscopically and through unit cell screening.[2] A small amount of precipitate was also observed, assumed to be $[Ca(H)Me]_\infty$.

Synthesis of $[(BDI)Ca(\mu\text{-}CH_3)_2Zn(\mu\text{-}H)]_2$ (3)

$ZnMe_2$ (1.0 M in heptane, 63.2 µl, 0.065 mmol) was added to a vial containing a toluene solution (*ca.* 2 cm^3) of $[(BDI)CaH]_2$ (30 mg, 0.033 mmol) and placed in the freezer (–35 °C), affording **3** as colourless crystals after 16 hours. The solution was decanted, and the crystals crushed and dried *in vacuo*. Yield: 34.4 mg, 94 %.

Upon solvation, at ambient temperature, **3** continues to react, ultimately affording [(BDI)ZnMe], however, this reaction does not proceed at –10 °C, the temperature at which the spectroscopic data was recorded.

^{1}H NMR (C_7D_8): δ = 7.10-7.06 (m, Ar-H, 2H), 6.78 (t, Ar-H, $^{3}J_{HH}$ = 3.2 Hz, 4H), 4.77 (s, HCCN, 1H), 3.22 (hept, $HC(CH_3)_2$, $^{3}J_{HH}$ = 6.82 Hz, 4H), 3.15 (s, Zn-H, 1H), 1.62 (s, $NCCH_3$, 6H), 1.18 (overlapping dd, $HC(CH_3)_2$, $^{3}J_{HH}$ = 6.82 Hz, 24 H), –0.66 (s, $Zn(\mu\text{-}CH_3)Ca$, 6H).

^{13}C{^{1}H} NMR (C_7D_8): δ = 166.6 ($NCCH_3$), 145.3 (*i*-C_6H_3), 141.7 (*o*-C_6H_3), 126.4 (*p*-C_6H_3), 124.0 (*m*-C_6H_3), 94.4 (HCCN), 28.5 ($HC(CH_3)_2$), 25.1 ($HC(CH_3)_2$), 24.6 ($HC(CH_3)_2$), 24.5 ($NCCH_3$), –6.6 (Zn-CH_3).

Anal. Calc. for $C_{62}H_{96}N_4Zn_2Ca_2$: C, 67.19; H, 8.73; N, 5.05. Found: C, 67.31; H, 8.32; N, 5.10.

Synthesis of [(BDI)CaMe]$_2$ (4)

$ZnMe_2$ (1.0 M in heptane, 16.3 μl, 0.016 mmol) was added to a toluene solution (*ca.* 2 cm^3) of [(BDI)CaH]$_2$ (30 mg, 0.03 mmol) and left to sit for 2 hours, after which time the volatiles were removed under reduced pressure, affording a crude yellow solid. The product was extracted into hexane and filtered into a vial before being placed in the freezer (–35 °C) for 16 hours. The solution was extracted away from the colourless crystals that formed overnight affording **4** with an associated molecule of hexane which cannot be removed under vacuum. Yield: 16.0 mg, 50 %.

^{1}H NMR (C_7D_8): δ = 7.06-7.02 (m, Ar-H, 2H), 6.80 (m, Ar-H, 4H), 4.69 (s, HCCN, 1H), 3.03 (hept, HC(CH_3)$_2$, $^3J_{HH}$ = 6.87 Hz, 4H), 1.57 (s, NCCH_3, 6H), 1.13 (d, HC(CH_3)$_2$, $^3J_{HH}$ = 6.87 Hz, 12H) , 0.97 (d, HC(CH_3)$_2$, $^3J_{HH}$ = 6.87 Hz, 12H), –1.36 (s, Ca-Me, 3H).

^{1}H NMR (C_6D_6): δ = 7.14-7.08 (m, Ar-H, 6H), 4.74 (s, HCCN, 1H), 3.08 (hept, HC(CH_3)$_2$, $^3J_{HH}$ = 6.87 Hz, 4H), 1.60 (s, NCCH_3, 6H), 1.14 (d, HC(CH_3)$_2$, $^3J_{HH}$ = 6.87 Hz, 12H), 1.00 (d, HC(CH_3)$_2$, $^3J_{HH}$ = 6.87 Hz, 12H), –1.29 (s, Ca-Me, 3H).

^{13}C{^{1}H} NMR (C_6D_6): δ = 166.1 (NCCH$_3$), 144.9 (*i*-C_6H_3), 142.1 (*o*-C_6H_3), 125.0 (*p*-C_6H_3), 124.3 (*m*-C_6H_3), 94.7 (HCCN), 28.4 (HC(CH_3)$_2$), 25.1 (HC(CH_3)$_2$), 24.7 (HC(CH_3)$_2$), 24.2 (NCCH_3), 8.3 (Ca-Me).

Anal. Calc. for $C_{60}H_{88}N_4Ca_2$: C, 76.22; H, 9.38; N, 5.93. Found: C, 77.07; H, 9.25; N, 6.05.

NMR Spectra

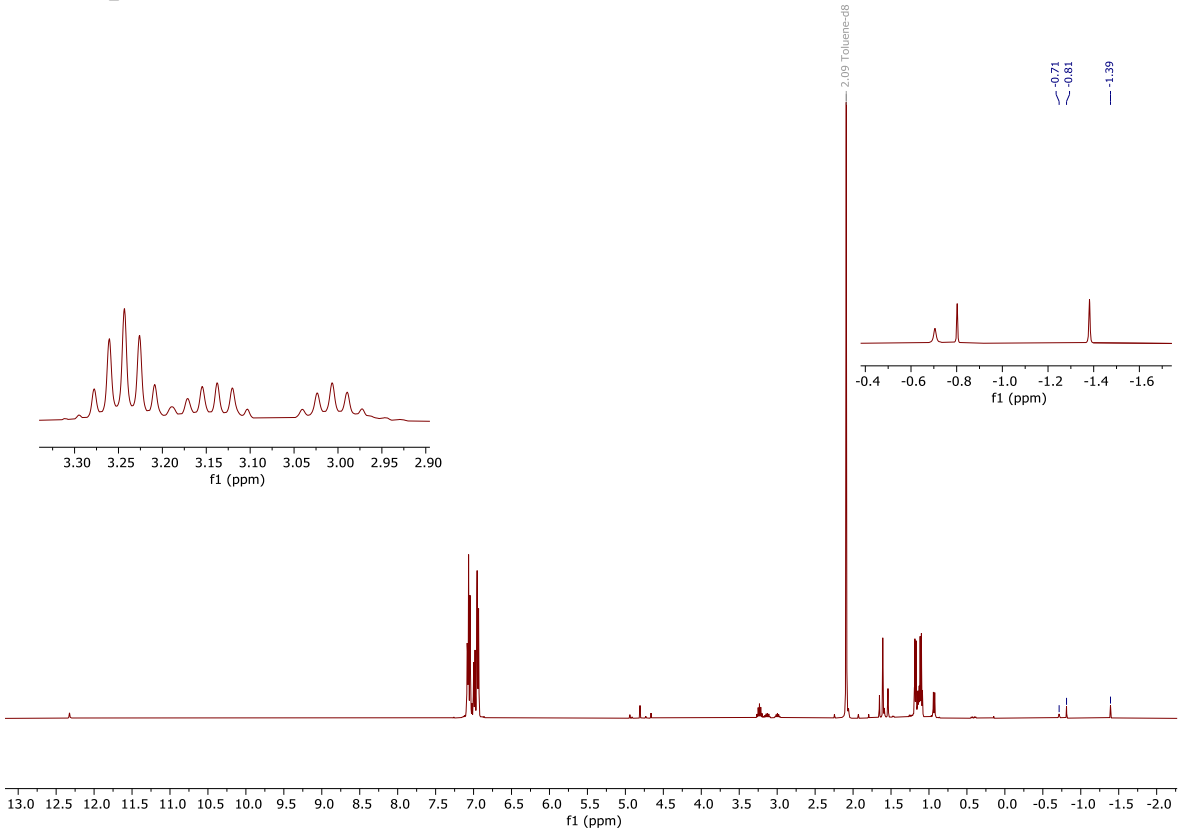

Figure S1. *^{1}H NMR Spectrum (C_7D_8, 298 K, 400.15 MHz) after removal of volatiles from reacting $[(BDI)CaH]_2$ with $ZnMe_2$.*

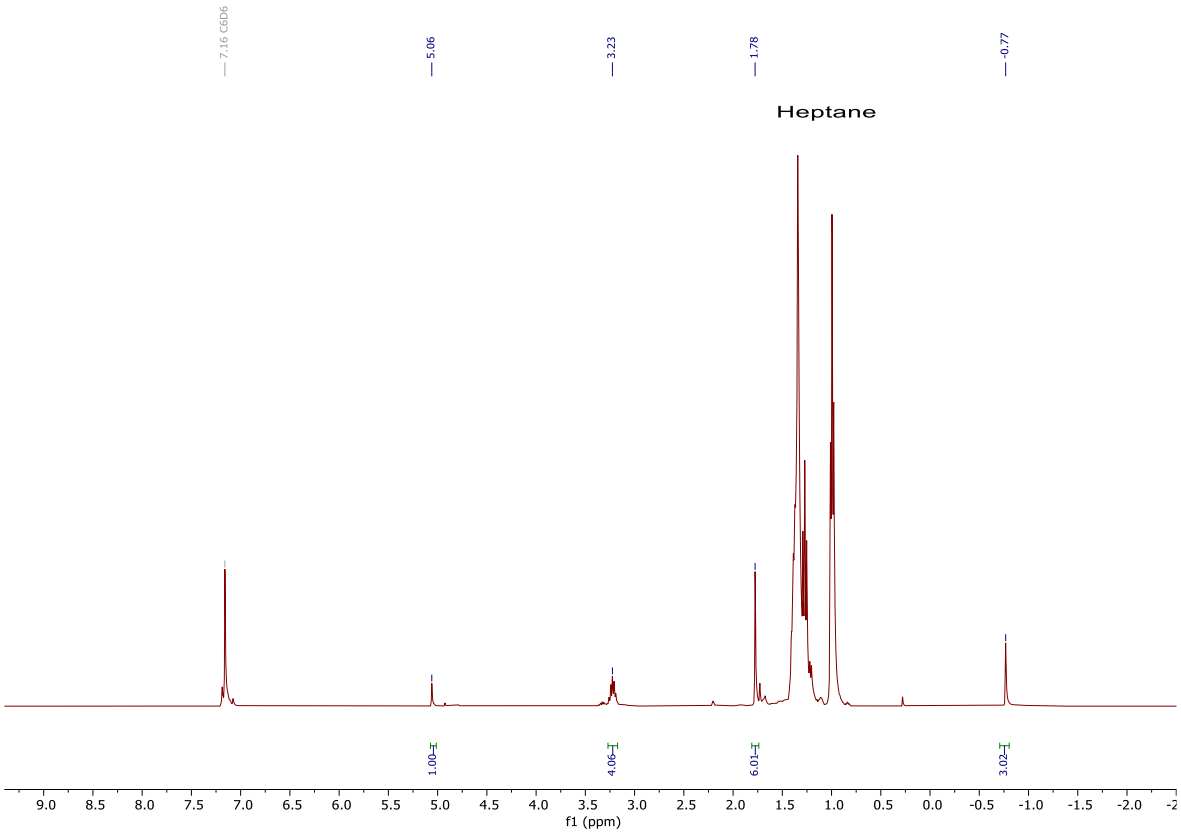

Figure S2. *^{1}H NMR Spectrum (C_6D_6, 298 K, 400.15 MHz) of [(BDI)ZnMe] from reacting $[(BDI)CaH]_2$ with 2 equiv. $ZnMe_2$.*

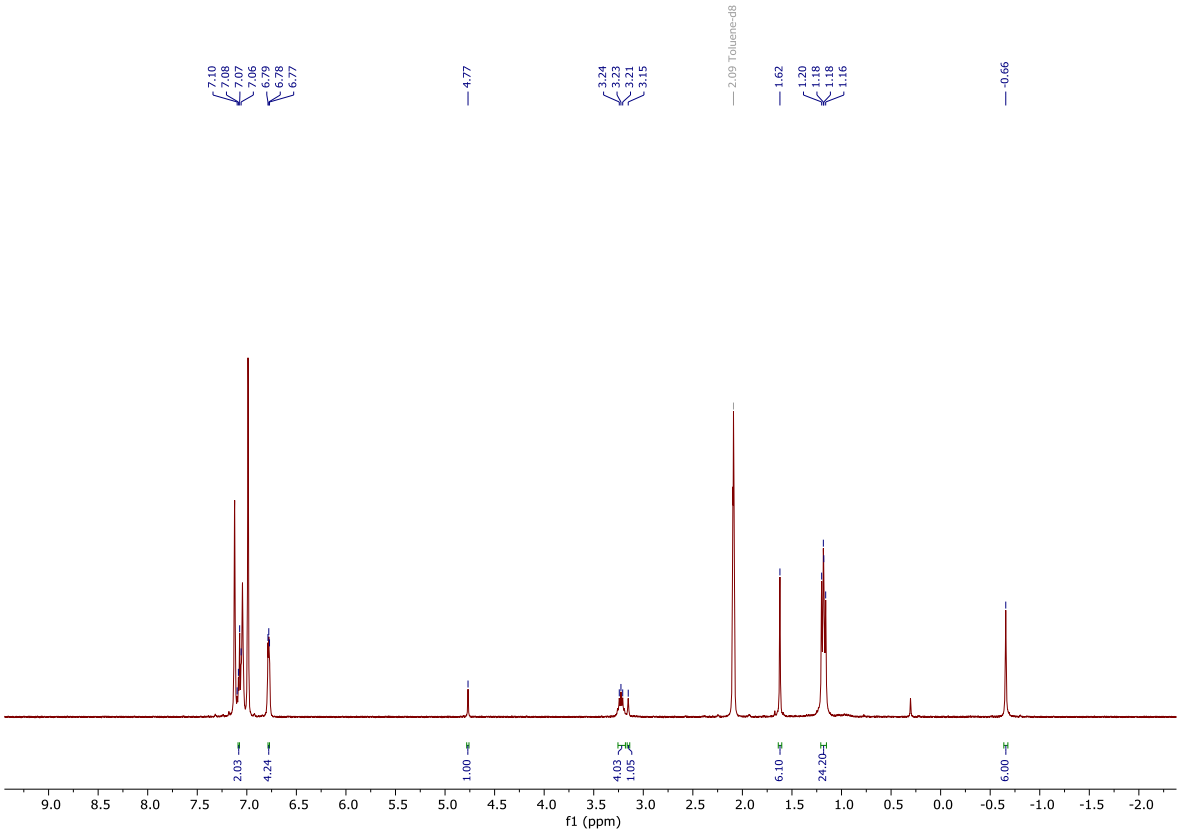

Figure S3. *^{1}H NMR Spectrum (C_7D_8, 263 K, 400.15 MHz) for* ***[(BDI)Ca(μ-CH$_3$)$_2$Zn(μ-H)]$_2$ (3)****.*

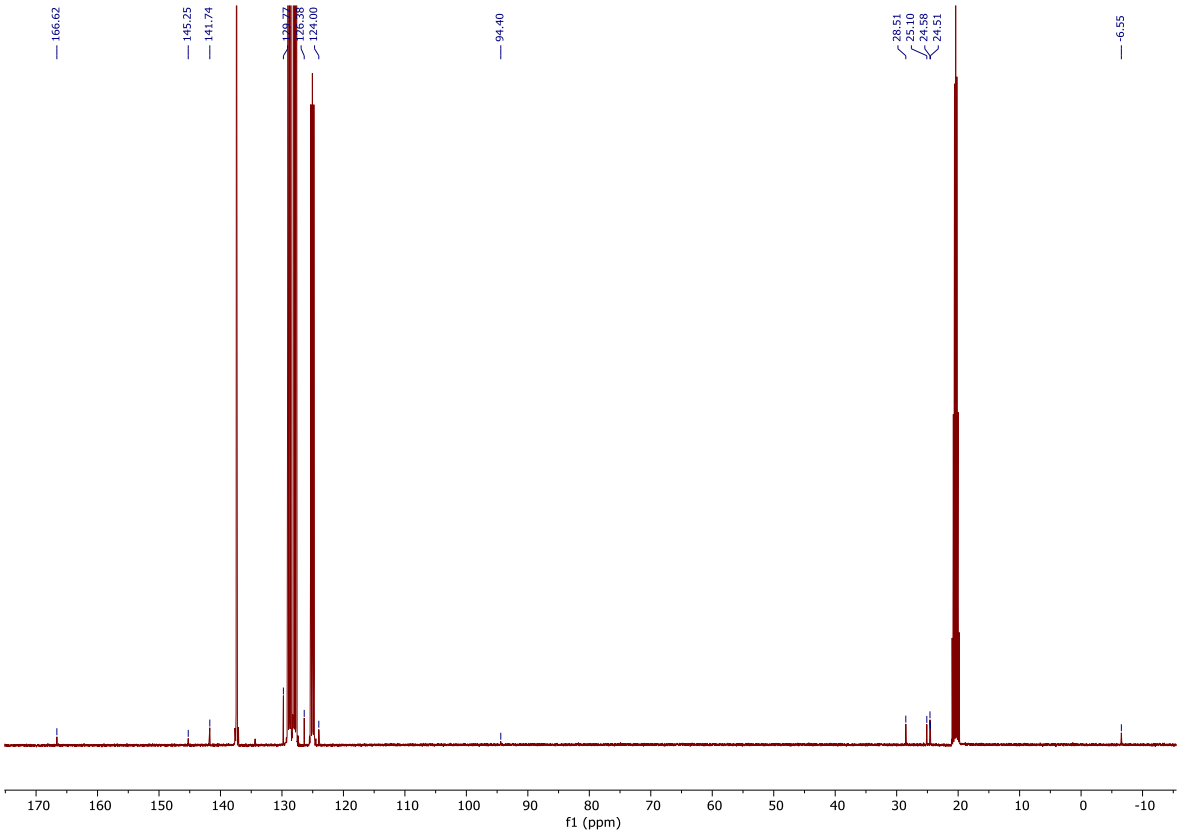

Figure S4. *^{13}C{^{1}H} NMR Spectrum (C_7D_8, 263 K, 100.62 MHz) for* ***[(BDI)Ca(μ-CH$_3$)$_2$Zn(μ-H)]$_2$ (3)****.*

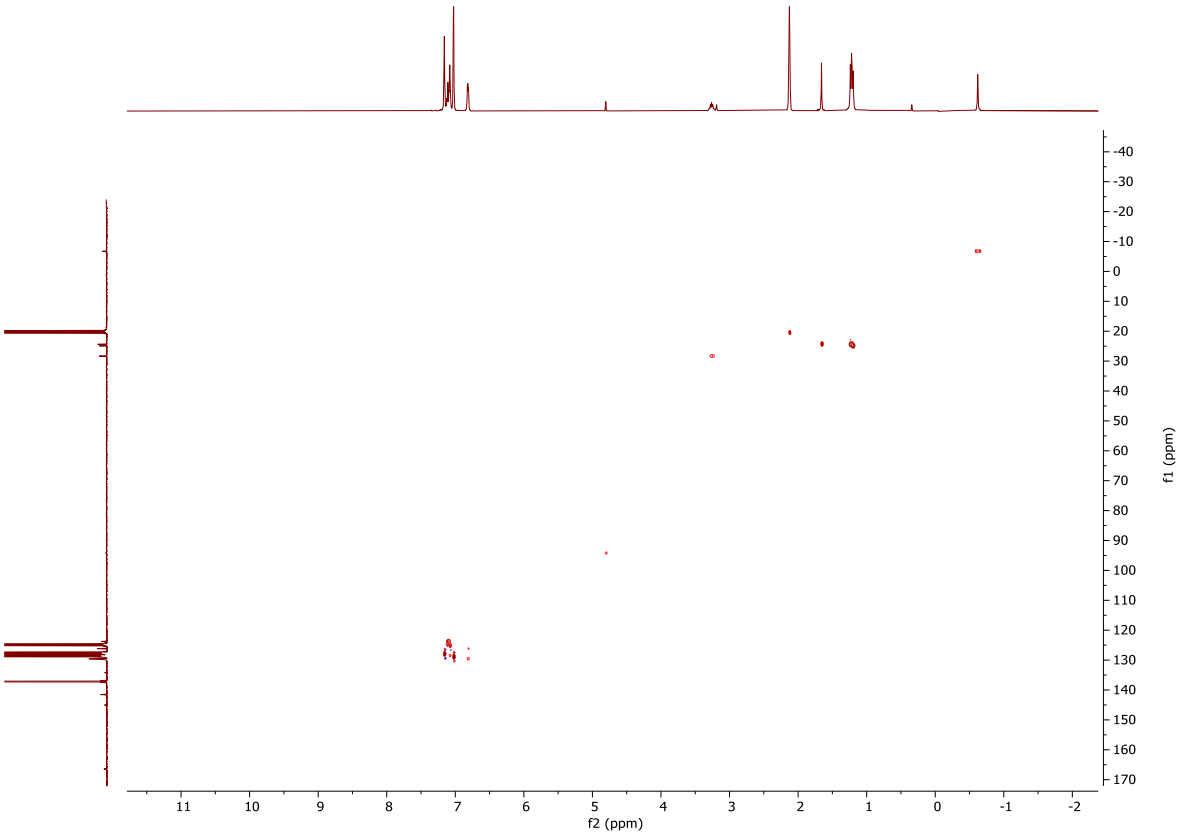

Figure S5. *^{1}H-^{13}C HSQC trace (C_7D_8, 263 K, 400.13, 100.62 MHz) for* ***[(BDI)Ca(μ-CH_3)$_2$Zn(μ-H)]$_2$ (3)***.

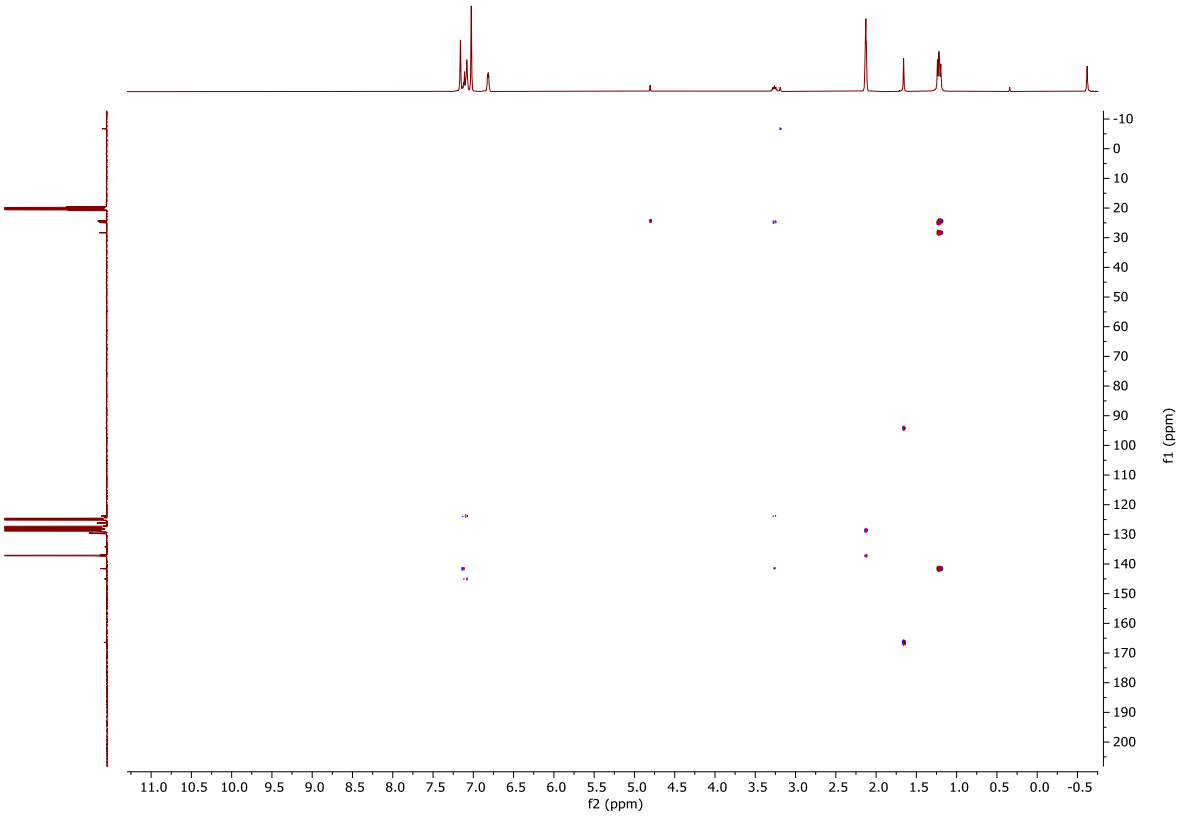

Figure S6. *^{1}H-^{13}C HMBC trace (C_7D_8, 263 K, 400.13, 100.62 MHz) for* ***[(BDI)Ca(μ-CH_3)$_2$Zn(μ-H)]$_2$ (3)***.

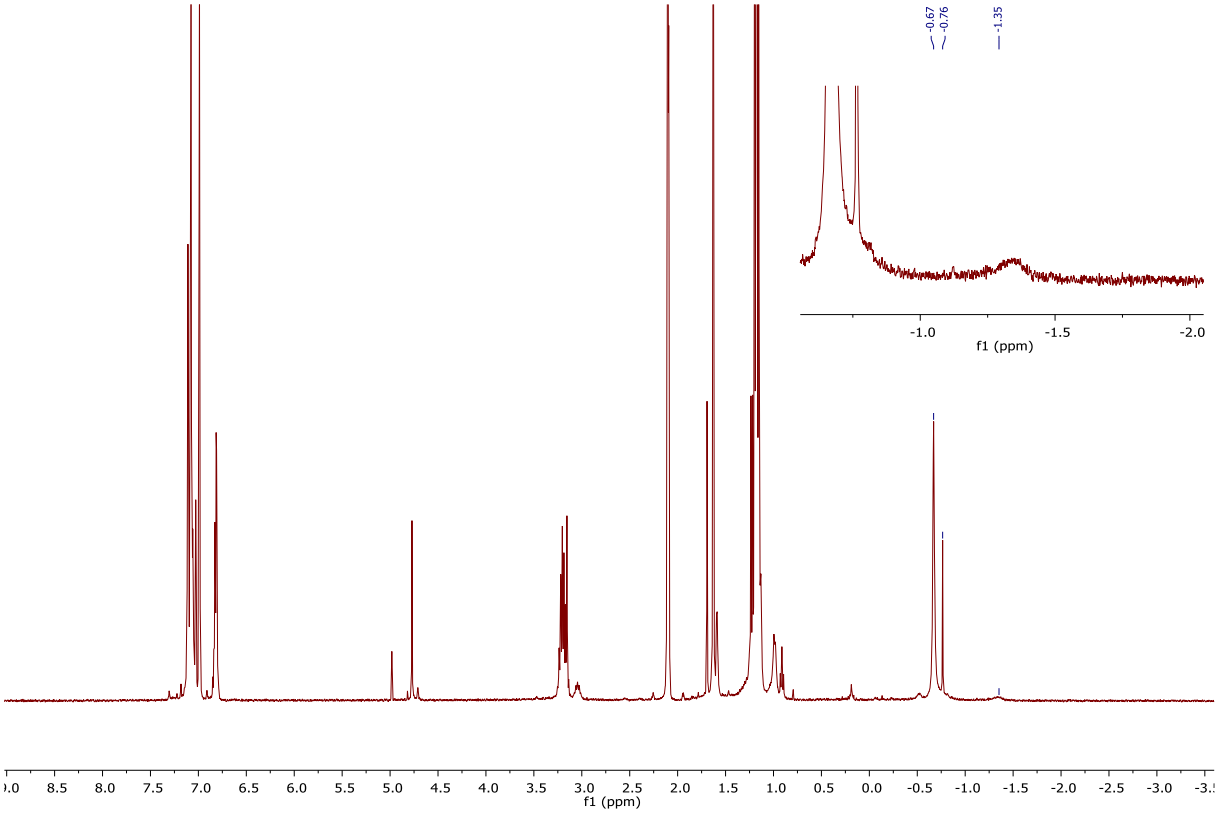

Figure S7. *^{1}H NMR Spectrum (C_7D_8, 298 K, 400.15 MHz) for* ***[(BDI)Ca(μ-CH$_3$)$_2$Zn(μ-H)]$_2$ (3)*** *after 2 hours.*

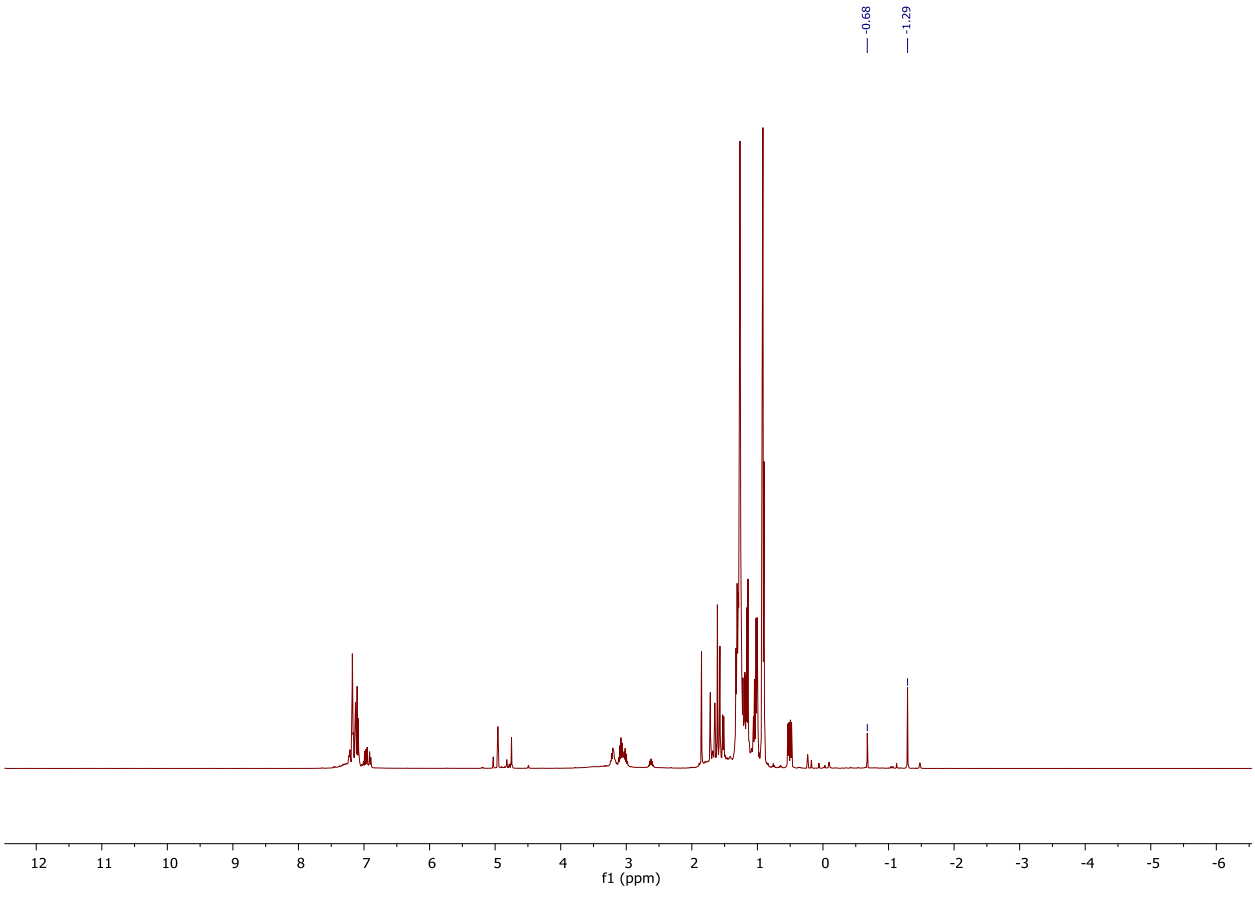

Figure S8. *^{1}H NMR Spectrum (C_6D_6, 298 K, 400.15 MHz) from reacting [(BDI)CaH]$_2$ and 0.5 ZnMe$_2$.*

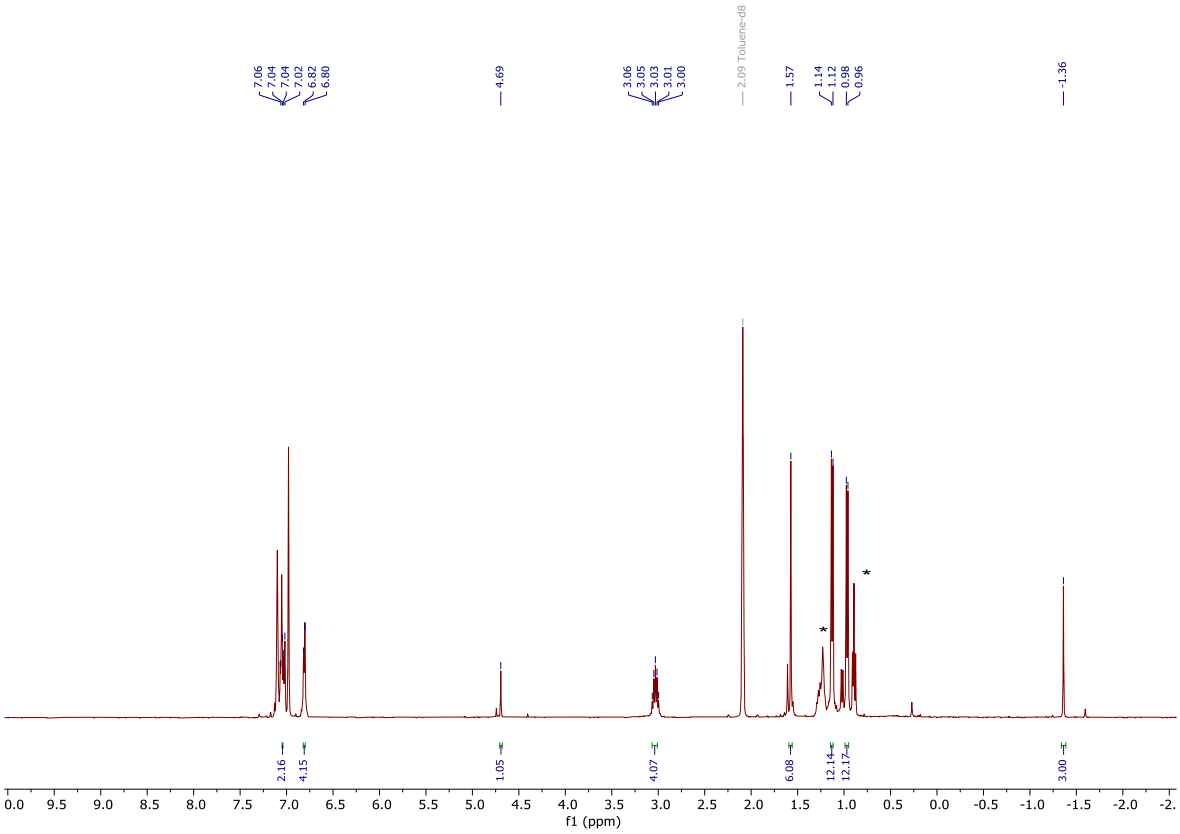

Figure S9. *^{1}H NMR Spectrum (C_7D_8, 298 K, 400.15 MHz) for* ***[(BDI)CaMe]$_2$ (4)****,* = Hexane.*

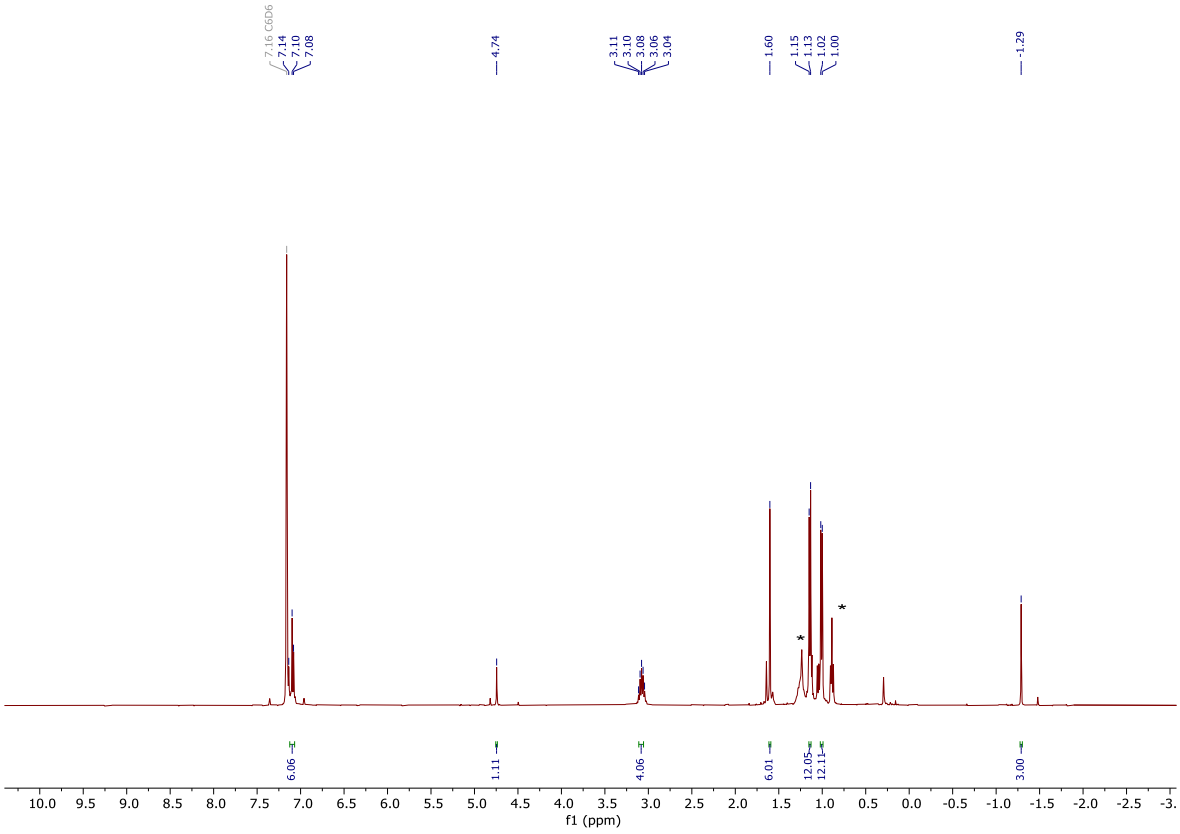

Figure 10. *^{1}H NMR Spectrum (C_6D_6, 298 K, 400.15 MHz) for* ***[(BDI)CaMe]$_2$ (4)****,* = Hexane.*

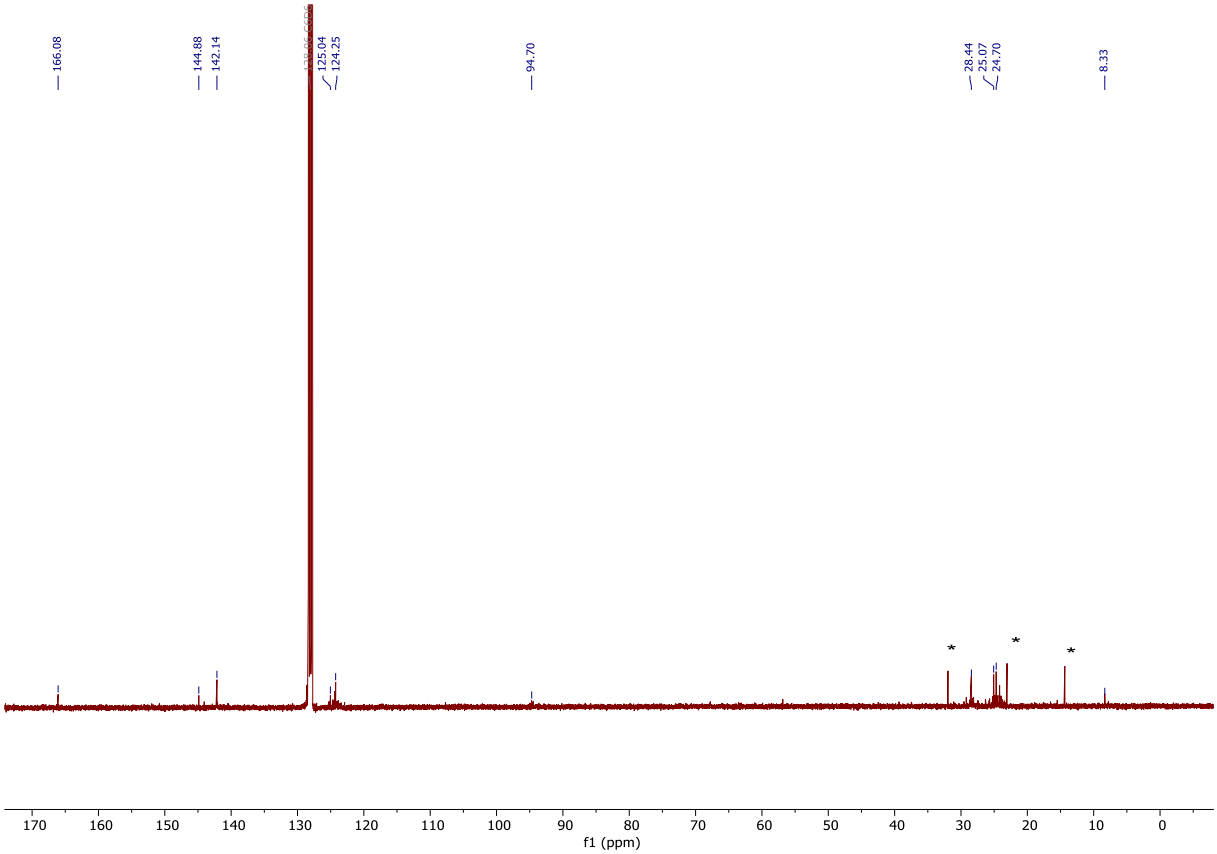

Figure S11. *$^{13}C\{^{1}H\}$ NMR Spectrum (C_6D_6, 298 K, 100.62 MHz) for* ***[(BDI)CaMe]$_2$ (4)****,* * = Hexane.*

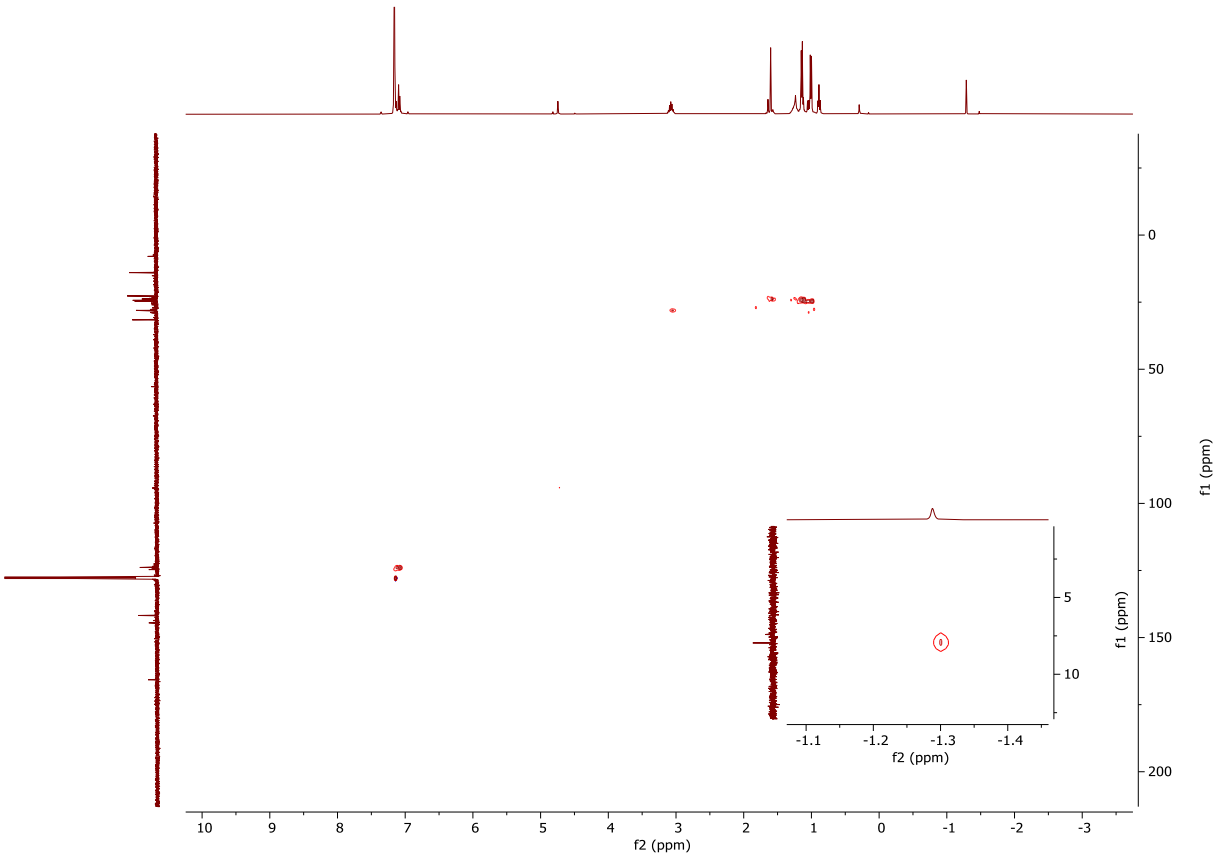

Figure S12. *^{1}H-^{13}C HSQC trace (C_6D_6, 298 K, 400.13, 100.62 MHz) for* ***[(BDI)CaMe]$_2$ (4)****.*

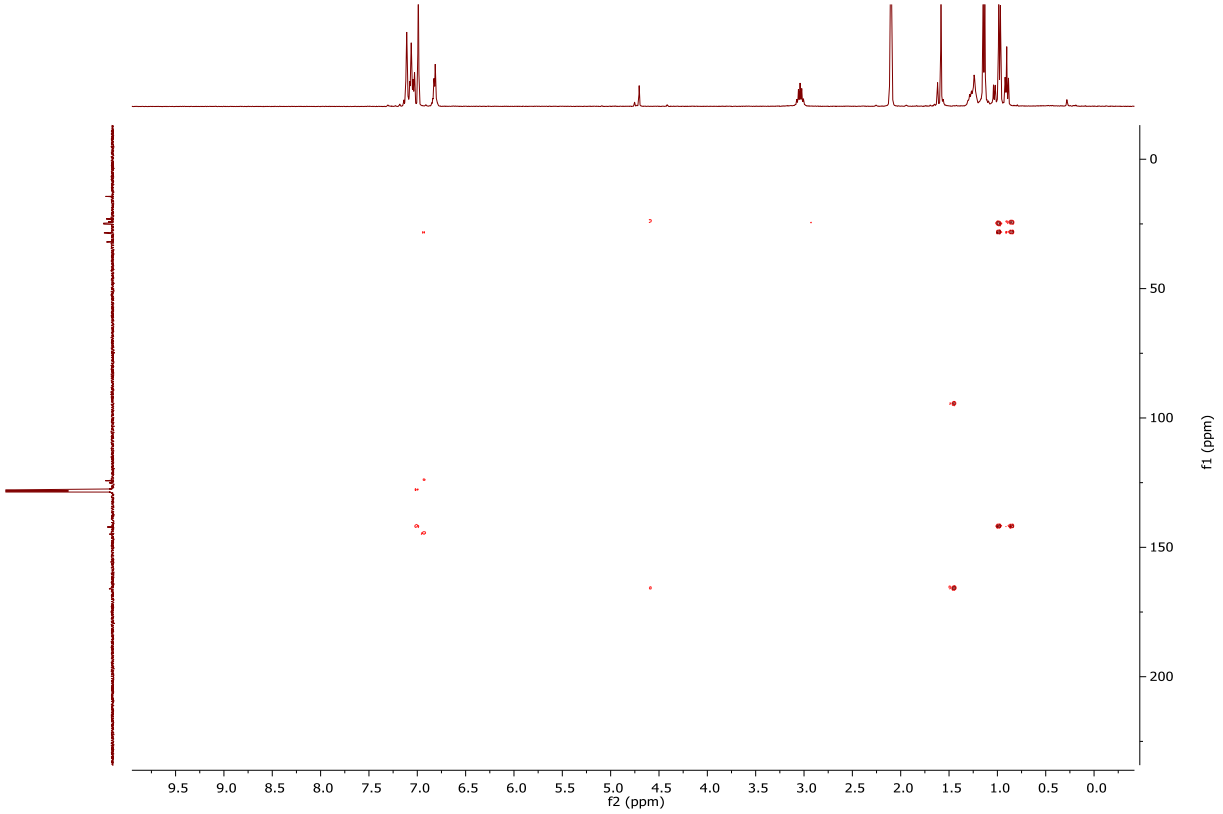

Figure S13. *^{1}H-^{13}C HMBC trace (C_6D_6, 298 K, 400.13, 100.62 MHz) for* ***[(BDI)CaMe]$_2$ (4)****.*

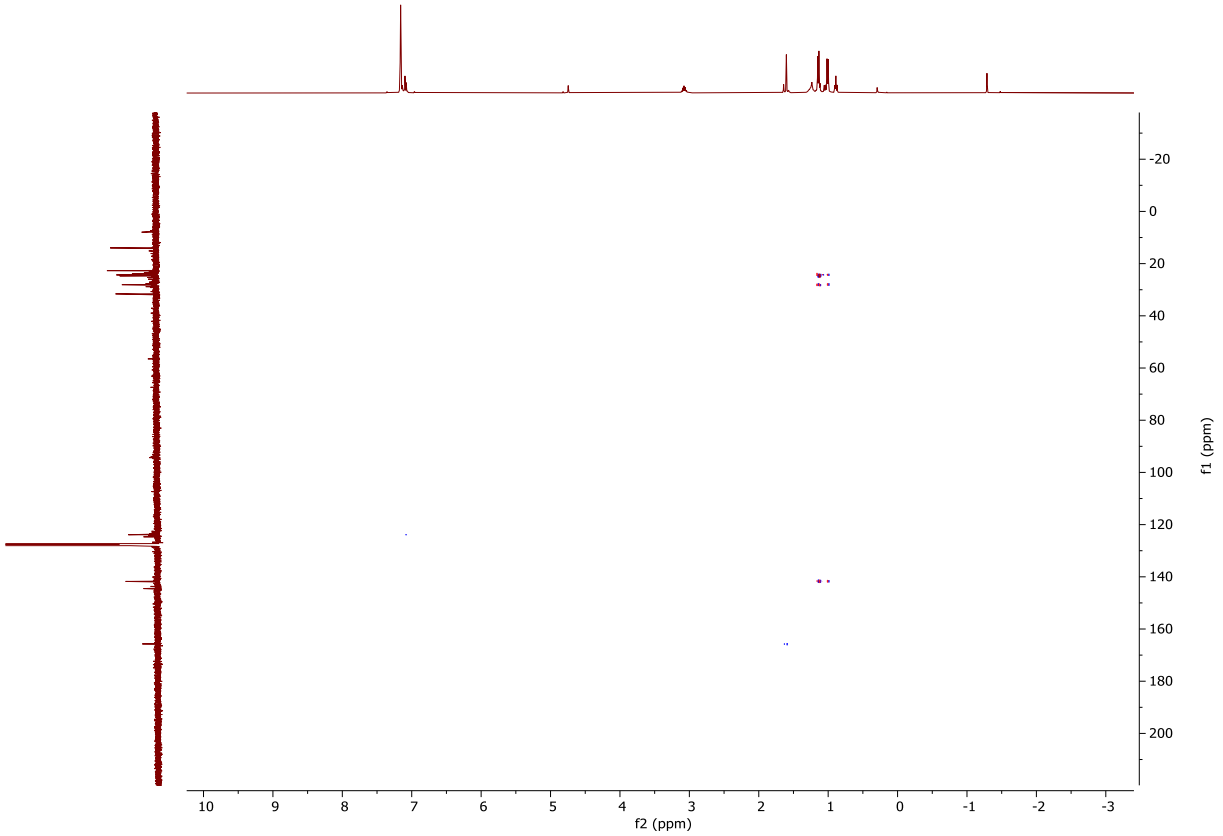

Figure S14. *^{1}H-^{13}C HMBC trace (C_6D_6, 298 K, 400.13, 100.62 MHz) for* ***[(BDI)CaMe]$_2$ (4)****.*

Crystallographic Details

Single Crystal X–ray diffraction data for compounds **3** – **4** were collected on an Agilent Xcalibur diffractomer using Mo-Kα radiation (λ = 0.71073 Å). In each case, the crystals were maintained at 150 K during data collection. Using Olex2,[3] the structures were solved with the olex2.solve[4] structure solution program or ShelXT and refined with the ShelXL[5] refinement package using Least−Squares minimisation.

The asymmetric unit in **3** contains two independent dimer halves and one molecule of benzene. Hydrogen atoms pertaining to the methyl groups containing C30, C31, C61 and C62 were located, and each refined at a distance of 0.98 Å from the relevant parent atom. Additionally, the hydrides (H1 and H2) were located and refined without restraints.

Large residual electron-density maxima proximate to both zinc centres could be equally well interpreted as either some metal disorder or data artifacts due to the deficiencies of the experiment itself.

The refinement presented here resolves all of these issues with the model, as presented, accounting for 95:05 disorder of both Zn1 and Zn2. The data quality actually permitted anisotropic refinement of the minor zinc portions without the inclusion of any restraints. Unsurprisingly, it was not feasible to locate a corresponding 5%, minor component, of the hydrides or the methyl groups based on C31 and C62. Scrutiny of the gross structure revealed a void (96 $Å^3$) that is centred at an average of the C16, C17, C59 and C60 positions and which is approximately co-planar with the included benzene moiety. However, the electron density calculation for this void suggests that there is in the region of 4 additional electrons present in the asymmetric unit. In fact, there is the ghost of a benzene molecule in this location, which could, with some restraints be modelled as 5% of an additional solvent molecule. While this modelling was not pursued, it would account for the zinc disorder observed and the concomitant effect that this would have, in terms of disorder, for C31 and C62.

The asymmetric unit in **4** contains half of a dimer molecule plus one molecule of hexane. The positions of H3a, H30b and H30c were assigned to the three largest electron-density maxima in the difference Fourier map, and these hydrogen positions were subsequently refined at a distance of 0.98Å from C30. The remainder of the dimer arises by virtue of crystallographic inversion symmetry.

Crystallographic data for all compounds have been deposited with the Cambridge Crystallographic Data Centre as supplementary publications CCDC 2360310-2360311 for **3** and **4**, respectively. Copies of these data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax(+44) 1223 336033], e-mail: deposit@ccdc.cam.ac.uk.

Table S1. *Crystal Data and Structure Refinement for Compounds **3** and **4**.*

Identification code	e24msh05 (**3**)	e24msh09 (**4**)
Empirical formula	$C_{136}H_{204}Ca_4N_8Zn_4$	$C_{72}H_{116}Ca_2N_4$
Formula weight	2372.86	1117.84
Crystal system	triclinic	monoclinic
Space group	*P*-1	$P2_1/n$
a/ Å	15.2503(6)	13.5951(4)
b/ Å	16.0371(6)	19.1092(4)
c/ Å	16.0776(6)	14.1535(4)
α/ °	69.051(4)	90
β/ °	69.699(4)	108.430(3)
γ/ °	71.172(4)	90
U/ Å^3	3354.3(3)	3488.37(17)
Z	1	2
ρ_{calc}/ g cm^{-3}	1.175	1.064
μ/ mm^{-1}	0.908	0.204
F(000)	1276.0	1232.0
Crystal size/ mm^3	0.538 × 0.388 × 0.226	0.405 × 0.319 × 0.188
2θ range for data collection/°	5.882 to 60.41	6.068 to 60.774
Index ranges	$-21 \le h \le 21$, $-22 \le k \le 16$, $-21 \le l \le 20$	$-18 \le h \le 18$, $-25 \le k \le 27$, $-13 \le l \le 20$
Reflections collected	32763	34856
Independent reflections, R_{int}	17073, 0.0277	9311, 0.0309
Data/restraints/parameters	17073/18/779	9311/4/376
Goodness–of–fit on F^2	1.026	1.030
Final *R*1, *wR*2 [$I>=2\sigma(I)$]	0.0439, 0.1154	0.0625, 0.1626
Final *R*1, *wR*2 [all data]	0.0631, 0.1289	0.0939, 0.1844
Largest diff. peak/hole/ e Å^{-3}	0.75/−0.70	0.91/−0.39

Computational Details

DFT calculations were run with Gaussian 16 (C.01).[6] The. Initial optimizations were performed with the TPSS[7] functional and def2-SVP[8] basis set for all atoms, using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as minima or transition states (by confirmation of all positive eigenvalues, or one imaginary eigenvalue respectively). Quantum Theory of Atoms in Molecules (QTAIM, AIMAll program[9]) and Natural Bonding Orbital (NBO7[10]) analyses were performed on the optimized geometries at the PBE0[11]/def2-TZVPP level of theory, with QTAIM values reported as atomic units throughout. To yield the reaction free energy profile for formation of **3**, energies were recomputed at the PBE0-D3BJ(CPCM=Benzene)/def2-TZVPP level using ORCA version 5.0.2,[12] with the CPCM model employed to incorporate benzene solvation effects ($\varepsilon = 2.2706$). This methodology was chosen as it was identified as an accurate performer in closed-shell organometallic reactivity[13] and barrier heights,[14] and general main-group kinetics and thermochemistry.[15]

Computed Mechanism for formation of 3

To survey the mechanistic steps involved in the of formation **3**, density functional theory (DFT) calculations were performed at the PBE0-D3BJ(CPCM=Benzene)/def2-TZVPP//TPSS/def2-SVP level of theory. The kinetically facile formation of **3** via addition of two equivalents of $ZnMe_2$ was envisaged to take place through three elementary steps which are presented in Figure S15. Initial addition of a first equivalent of $ZnMe_2$ proceeds with Zn–H coupling, and a concomitant σ-coordination of the methyl group with a Ca(II) center *via* low-lying saddle point **TS(I-II)** (+6.7 kcal mol^{-1}) to exergonically afford **II** (–7.0 kcal mol^{-1}). Corresponding Ca–H elongation (**I**: 2.15 Å, **II**: 2.47 Å) at the participating hydride along with formation of a short Zn···H contact (1.73 Å) indicates the first step consists of a hydride transfer to the electrophilic Zn(II) center. Addition of a second equivalent of $ZnMe_2$ subsequently takes place at the other coordinatively unsaturated hydride with initial σ-coordination of $ZnMe_2$ to the Ca centre *via* the Me group to form **III** (+1.5 kcal mol^{-1}), which is then followed by Zn–H coupling at **TS(III-IV)** (+3.2 kcal mol^{-1}) to form **IV** (–11.9 kcal mol^{-1}) which, also leads to Ca–H elongation with respect to the participating hydride. Finally, rearrangement of **IV** leads to the formation of two complementary bridging Zn–H–Zn interactions, ultimately forming the observed product **V** (**3**, –16.0 kcal mol^{-1}) via **TS(IV-V)** (–7.4 kcal mol^{-1}).

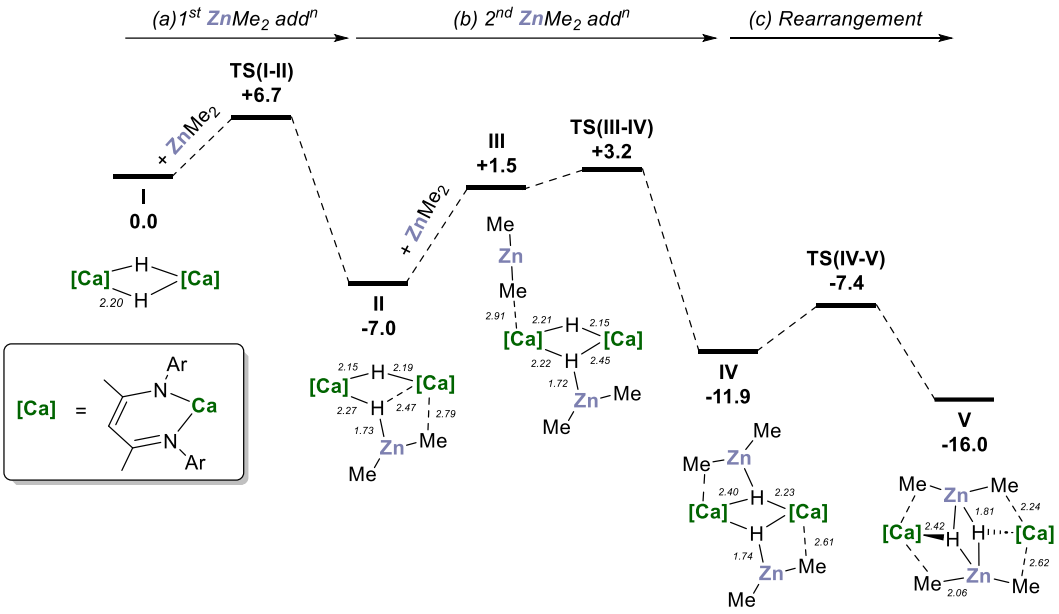

Figure S15. *Free energy profile (calculated with DFT at the PBE0-D3BJ(CPCM=Benzene)/def2-TZVPP//TPSS/def2-SVP level of theory, energies in kcal mol^{-1}) for the addition of $ZnMe_2$ to* ***I*** *to form* ***V*** */* ***3****.*

Breakdown of energy contributions

The following table details the evolution of the relative energies as the successive corrections to the initial SCF energy are included. Terms used are:

$\mathbf{\Delta E_{BSI}}$	SCF energy computed with the TPSS functional with def2-SVP
$\mathbf{\Delta H_{BSI}}$	Enthalpy at 0 K with def2-SVP
$\mathbf{\Delta G_{BSI}}$	Free energy at 298.15 K and 1 atm with def2-SVP
$\mathbf{\Delta E_{PBE0-D3/C_6H_6/BS2}}$	SCF energy computed with PBE0-D3BJ;CPCM(Benzene)/def2-TZVPP
$\mathbf{\Delta G_{PBE0-D3/C_6H_6/BS2}}$	Free energy computed at the PBE0-D3BJ;CPCM(Benzene)/def2-TZVPP//TPSS/def2-SVP level

In each case the final data used in the main article are highlighted in bold.

Table S2. *Relative energies (kcal mol^{-1}) for computed structures. Data in bold are those used in the main text. All energies are quoted relative to* ***I*** *at 0.0 kcal/mol.*

	ΔE_{BSI}	ΔH_{BSI}	ΔG_{BSI}	$\Delta E_{PBE0-D3/C_6H_6/BS2}$	$\Delta G_{PBE0-D3/C_6H_6/BS2}$
I	0.0	0.0	0.0	0.0	**0.0**
TS(I-II)	-1.3	-0.8	11.8	-6.4	**6.7**
II	-13.6	-12.3	-1.3	-19.3	**-7.0**
TS(II-III)	-11.4	-8.7	17.4	-27.3	**1.5**
III	-10.7	-8.5	19.9	-27.4	**3.2**
TS(III-IV)	-26.7	-23.7	4.4	-42.9	**-11.9**
IV	-25.6	-23.3	7.6	-40.6	**-7.4**
TS(IV-V)	-44.1	-41.1	-12.8	-47.2	**-16.0**

QTAIM and NBO data of calculated structures 1, 3, 4 and $ZnMe_2$

Table S3. *Selected QTAIM BCP data for* ***3****.*

BCP	**ρ(r)**	**$\nabla^2\rho(r)$**	**ε**	**G(r)**	**V(r)**	**H(r)**
Ca1 - C77	0.024173	0.095699	0.358634	-0.01994	0.021932	0.001993
Ca1 - H165	0.02136	0.06216	0.184949	-0.01492	0.01523	0.00031
Ca1 - C162	0.024186	0.096871	0.288364	-0.02009	0.022156	0.002062
Zn83 - H165	0.062984	0.161535	0.07102	-0.06621	0.053296	-0.01291
C77 - Zn83	0.086999	0.218216	0.087662	-0.10288	0.078719	-0.02417
H82 - Zn83	0.062647	0.160554	0.072035	-0.06576	0.052949	-0.01281
C79 - Zn83	0.087582	0.219322	0.086745	-0.10393	0.079382	-0.02455
C79 - Ca84	0.024186	0.096871	0.288364	-0.02009	0.022156	0.002062
H82 - Ca84	0.02136	0.06216	0.184949	-0.01492	0.01523	0.00031
H82 - Zn166	0.062984	0.161535	0.07102	-0.06621	0.053296	-0.01291
Ca84 - C160	0.024173	0.095699	0.358634	-0.01994	0.021932	0.001993
C162 - Zn166	0.087582	0.219322	0.086745	-0.10393	0.079382	-0.02455
C160 - Zn166	0.086999	0.218216	0.087662	-0.10288	0.078719	-0.02417
H165 - Zn166	0.062647	0.160554	0.072035	-0.06576	0.052949	-0.01281

***Table S4**. Selected donor acceptor interaction energies, $\Delta E^{(2)}$ in **3**.*

Donor NBO unit	Acceptor NBO unit	$\Delta E^{(2)}$ (kcal mol^{-1})
LP_{C77}	n_{Ca1}*	2.63
$\sigma_{C77–H2}$	n_{Ca1}*	1.36
$\sigma_{C77–H3}$	n_{Ca1}*	1.36
LP_{C77}	n_{Zn83}*	94.84
LP_{C79}	n_{Ca84}*	2.64
$\sigma_{C79–H4}$	n_{Ca84}*	1.49
$\sigma_{C79–H80}$	n_{Ca84}*	1.49
LP_{C79}	n_{Zn83}*	96.04
LP_{H82}	n_{Zn83}*	79.59
LP_{H82}	n_{Ca84}*	4.75
LP_{H82}	n_{Zn166}*	79.19
LP_{C160}	n_{Ca84}*	2.63
$\sigma_{C160–H85}$	n_{Ca84}*	1.36
$\sigma_{C160–H86}$	n_{Ca84}*	1.36
LP_{C160}	n_{Zn166}*	94.84
LP_{C162}	n_{Ca1}*	2.64
$\sigma_{C162–H87}$	n_{Ca1}*	1.49
$\sigma_{C162–H164}$	n_{Ca1}*	1.49
LP_{C162}	n_{Zn166}*	96.04
LP_{H165}	n_{Ca1}*	4.75
LP_{H165}	n_{Zn83}*	79.19
LP_{H165}	n_{Zn166}*	79.59

***Table S4.** Selected QTAIM BCP data for **1**.*

BCP	ρ(r)	$\nabla^2\rho(r)$	ε	G(r)	V(r)	H(r)
Ca1 - H2	0.032163	0.081947	0.003544	-0.02387	0.022177	-0.00169
Ca75 - H76	0.032163	0.081947	0.003544	-0.02387	0.022177	-0.00169
Ca1 - H76	0.03258	0.083485	0.005376	0.001697	-0.02426	0.022568
H2 - Ca75	0.03258	0.083485	0.005376	0.001697	-0.02426	0.022568

***Table S5.** Selected QTAIM BCP data for **4**.*

BCP	ρ(r)	$\nabla^2\rho(r)$	ε	G(r)	V(r)	H(r)
Ca1 - C42	0.033841	0.109728	0.076368	-0.02825	0.027842	-0.00041
Ca78 - C119	0.033835	0.10966	0.077401	-0.02824	0.027827	-0.00041
Ca1 - C119	0.033947	0.099452	0.126371	-0.02696	0.025909	-0.00105
C42 - Ca78	0.033947	0.099423	0.126174	-0.02695	0.025903	-0.00105

***Table S6.** Selected QTAIM atomic data for **4**.*

Name	q(A)
Ca1	1.592666
C42	-0.639997
Ca78	1.592741
C119	-0.640009

Table S7. *Selected QTAIM BCP data for* ***$ZnMe_2$****.*

BCP	**ρ(r)**	**$\nabla^2\rho(r)$**	**ε**	**G(r)**	**V(r)**	**H(r)**
C4 - Zn9	0.113551	0.209903	0.000026	-0.14308	0.097777	-0.0453
C6 - Zn9	0.113551	0.209903	0.000036	-0.14308	0.097777	-0.0453

Cartesian Coordinates and Computed Energies (in Hartrees) for Calculated Structures

$ZnMe_2$
SCF (TPSS/SVP) Energy = -1858.92128416
Enthalpy 298K = -1858.845034
Free Energy 298K = -1858.882464
Lowest Frequency = 12.2337 cm^{-1}
Second Frequency = 134.5122 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -1858.898279774258

H	2.35887	-0.49538	0.90273
H	2.35805	-0.53511	-0.88080
H	-2.35802	-0.53643	-0.87999
C	1.95353	-0.00015	-0.00031
H	2.35900	1.02947	-0.02339
C	-1.95353	-0.00014	-0.00030
H	-2.35910	1.02940	-0.02495
H	-2.35880	-0.49412	0.90346
Zn	0.00000	0.00013	0.00022

I
SCF (TPSS/SVP) Energy = -3833.75394321
Enthalpy 298K = -3832.414653
Free Energy 298K = -3832.611887
Lowest Frequency = 8.4175 cm^{-1}
Second Frequency = 15.8777 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -3832.890938

Ca	0.16221	-0.40178	-1.70057
H	1.12797	-0.65638	0.26759
N	-0.46086	-2.10145	-3.22503
N	1.13748	0.46240	-3.67527
C	-0.52304	-3.52846	-5.24184
H	-0.26850	-4.45057	-4.69148
H	-0.07925	-3.57961	-6.24754
H	-1.62288	-3.51943	-5.34107
C	-0.04679	-2.29591	-4.48694
C	0.79805	-1.41404	-5.20521
H	1.04599	-1.74638	-6.21699
C	1.30083	-0.13345	-4.86684
C	2.05141	0.60262	-5.96712
H	1.53316	1.54287	-6.22575
H	2.13811	-0.01298	-6.87514
H	3.06318	0.88811	-5.63109
C	-1.39945	-3.00761	-2.63647
C	-2.79663	-2.72295	-2.71557
C	-3.33055	-1.54704	-3.53785
H	-2.46720	-1.08891	-4.05064
C	-4.32409	-2.00738	-4.62683
H	-3.87695	-2.77079	-5.28714
H	-4.63145	-1.15091	-5.25399
H	-5.23886	-2.44131	-4.18370
C	-3.96911	-0.46253	-2.64312
H	-4.84659	-0.85859	-2.10036
H	-4.30911	0.39324	-3.25437
H	-3.25630	-0.08246	-1.88980
C	-3.69786	-3.55633	-2.02788
H	-4.77203	-3.34323	-2.08225
C	-3.25232	-4.65210	-1.28129
H	-3.96988	-5.28656	-0.74960
C	-1.88392	-4.93617	-1.22400
H	-1.53893	-5.80038	-0.64491
C	-0.93980	-4.13774	-1.89515
C	0.54600	-4.49924	-1.82310
H	1.07733	-3.84264	-2.53413
C	0.81283	-5.95817	-2.25270
H	1.89952	-6.15671	-2.27935
H	0.40176	-6.16890	-3.25562
H	0.36130	-6.67896	-1.54722
C	1.13003	-4.23174	-0.41935
H	1.02777	-3.17119	-0.12708
H	2.20558	-4.48590	-0.39081
H	0.61523	-4.83881	0.34696
C	1.60124	1.80208	-3.47929
C	2.91706	2.04128	-2.97977
C	3.91801	0.90060	-2.77819

H	3.47199	-0.00787	-3.21947
C	5.25368	1.16125	-3.50784
H	5.79194	2.02396	-3.07524
H	5.09768	1.36790	-4.58125
H	5.91526	0.28045	-3.42125
C	4.16474	0.61587	-1.28113
H	4.88003	-0.21786	-1.15673
H	3.23261	0.33954	-0.75630
H	4.58263	1.50308	-0.77213
C	3.29578	3.36189	-2.67661
H	4.30066	3.55371	-2.28344
C	2.41882	4.43469	-2.86794
H	2.73429	5.45491	-2.62355
C	1.13936	4.19599	-3.38036
H	0.45854	5.04002	-3.54257
C	0.70779	2.89471	-3.69685
C	-0.69312	2.68215	-4.27682
H	-0.78407	1.61062	-4.52543
C	-0.90470	3.47916	-5.58253
H	-0.86861	4.56902	-5.40258
H	-1.89254	3.24601	-6.01972
H	-0.13316	3.23793	-6.33436
C	-1.79769	3.01691	-3.25100
H	-1.69379	2.41842	-2.32848
H	-2.79700	2.81577	-3.67818
H	-1.76356	4.08287	-2.96117
Ca	-0.16221	0.40178	1.70057
H	-1.12797	0.65638	-0.26759
N	0.46086	2.10145	3.22503
N	-1.13748	-0.46240	3.67527
C	0.52304	3.52846	5.24184
H	0.26850	4.45057	4.69148
H	0.07925	3.57961	6.24754
H	1.62288	3.51943	5.34107
C	0.04679	2.29591	4.48694
C	-0.79805	1.41404	5.20521
H	-1.04599	1.74638	6.21699
C	-1.30083	0.13345	4.86684
C	-2.05141	-0.60262	5.96712
H	-1.53316	-1.54287	6.22575
H	-2.13811	0.01298	6.87514
H	-3.06318	-0.88811	5.63109
C	1.39945	3.00761	2.63647
C	2.79663	2.72295	2.71557
C	3.33055	1.54704	3.53785
H	2.46720	1.08891	4.05064
C	4.32409	2.00738	4.62683
H	3.87695	2.77079	5.28714
H	4.63145	1.15091	5.25399
H	5.23886	2.44131	4.18370
C	3.96911	0.46253	2.64312
H	4.84659	0.85859	2.10036
H	4.30911	-0.39324	3.25437
H	3.25630	0.08246	1.88980
C	3.69786	3.55633	2.02788
H	4.77203	3.34323	2.08225
C	3.25232	4.65210	1.28129
H	3.96988	5.28656	0.74960
C	1.88392	4.93617	1.22400
H	1.53893	5.80038	0.64491
C	0.93980	4.13774	1.89515
C	-0.54600	4.49924	1.82310
H	-1.07733	3.84264	2.53413
C	-0.81283	5.95817	2.25270
H	-1.89952	6.15671	2.27935
H	-0.40176	6.16890	3.25562
H	-0.36130	6.67896	1.54722
C	-1.13003	4.23174	0.41935
H	-1.02777	3.17119	0.12708
H	-2.20558	4.48590	0.39081
H	-0.61523	4.83881	-0.34696
C	-1.60124	-1.80208	3.47929
C	-2.91706	-2.04128	2.97977
C	-3.91801	-0.90060	2.77819
H	-3.47199	0.00787	3.21947
C	-5.25368	-1.16125	3.50784
H	-5.79194	-2.02396	3.07524

H -5.09768 -1.36790 4.58125
H -5.91526 -0.28045 3.42125
C -4.16474 -0.61587 1.28113
H -4.88003 0.21786 1.15673
H -3.23261 -0.33954 0.75630
H -4.58263 -1.50308 0.77213
C -3.29578 -3.36189 2.67661
H -4.30066 -3.55371 2.28344
C -2.41882 -4.43469 2.86794
H -2.73429 -5.45491 2.62355
C -1.13936 -4.19599 3.38036
H -0.45854 -5.04002 3.54257
C -0.70779 -2.89471 3.69685
C   0.69312 -2.68215 4.27682
H   0.78407 -1.61062 4.52543
C   0.90470 -3.47916 5.58253
H   0.86861 -4.56902 5.40258
H   1.89254 -3.24601 6.01972
H   0.13316 -3.23793 6.33436
C   1.79769 -3.01691 3.25100
H   1.69379 -2.41842 2.32848
H   2.79700 -2.81577 3.67818
H   1.76356 -4.08287 2.96117

TS(I-II)
SCF (TPSS/SVP) Energy = -5692.67736902
Enthalpy 298K = -5691.260957
Free Energy 298K = -5691.475588
Lowest Frequency = -22.9633 cm^{-1}
Second Frequency = 10.3704 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -5691.799492

Ca 1.68284 -0.48369 -0.05459
N   2.96009 -2.39188 -0.60317
N   3.83598 0.48003 0.12897
C   4.28164 -2.56562 -0.44123
C   5.19127 -1.55353 -0.04408
H   6.22739 -1.89164 0.04350
C   5.01732 -0.15943 0.14469
C   4.89088 -3.92999 -0.73107
H   5.96980 -3.94168 -0.51501
H   4.73952 -4.20467 -1.78976
H   4.39746 -4.71550 -0.13311
C   6.29450 0.64576 0.33779
H   6.25821 1.23401 1.27010
H   6.41555 1.37365 -0.48407
H   7.17984 -0.00714 0.36252
C   2.17330 -3.44956 -1.16547
C   1.52920 -4.39834 -0.31679
C   0.68464 -5.36404 -0.89484
H   0.18201 -6.09157 -0.24737
C   0.47635 -5.41695 -2.27659
H -0.18241 -6.17925 -2.70702
C   1.11784 -4.48963 -3.10427
H   0.95619 -4.53381 -4.18776
C   1.96710 -3.49928 -2.57774
C   1.72730 -4.38269 1.19985
H   2.53234 -3.65932 1.41953
C   2.17565 -5.75270 1.75212
H   3.08624 -6.11648 1.24460
H   1.39089 -6.52005 1.62409
H   2.39254 -5.67666 2.83278
C   0.45231 -3.89828 1.92229
H -0.40479 -4.55958 1.70396
H   0.16631 -2.87811 1.60735
H   0.60576 -3.87819 3.01531
C   2.64351 -2.50927 -3.52916
H   3.28356 -1.85090 -2.91658
C   1.60885 -1.61741 -4.25007
H   0.98172 -1.06377 -3.52934
H   0.93722 -2.22105 -4.88762
H   2.11821 -0.88334 -4.90081
C   3.55622 -3.22084 -4.55184
H   2.97416 -3.87673 -5.22466
H   4.31802 -3.84435 -4.05229
H   4.08158 -2.47907 -5.18049
C   3.80520 1.90904 0.22637

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C   3.75590  2.55077  1.50121
C   3.63722  3.95202  1.55116
H   3.60083  4.45062  2.52686
C   3.56613  4.72194  0.38558
H   3.47370  5.81181  0.44788
C   3.61661  4.08804 -0.85969
H   3.56272  4.69168 -1.77304
C   3.74018  2.69063 -0.96727
C   3.82530  1.76075  2.81042
H   4.02033  0.70556  2.55110
C   4.97414  2.23699  3.72605
H   4.81027  3.27195  4.07676
H   5.94775  2.21046  3.20649
H   5.04566  1.59005  4.61889
C   2.48163  1.81476  3.56962
H   1.65675  1.40407  2.95922
H   2.21455  2.85354  3.83463
H   2.54654  1.23196  4.50687
C   3.81555  2.04966 -2.35517
H   3.95280  0.96416 -2.20724
C   2.50872  2.25503 -3.15158
H   2.30433  3.32776 -3.31869
H   1.63682  1.83020 -2.62331
H   2.57717  1.76533 -4.13987
C   5.03127  2.56090 -3.15909
H   5.97593  2.40126 -2.61065
H   4.94681  3.64141 -3.37573
H   5.10384  2.03065 -4.12597
H   0.00025  0.00007 -1.34979
Ca -1.68240  0.48365 -0.05462
H  -2.00520  1.32559  5.74719
H  -1.80026  1.67738  4.01107
H   1.99941 -1.32420  5.75191
N  -2.95956  2.39188 -0.60325
N  -3.83552 -0.48014  0.12863
C  -4.28108  2.56565 -0.44106
C  -5.19069  1.55355 -0.04386
H  -6.22678  1.89171  0.04394
C  -5.01682  0.15940  0.14458
C  -4.89035  3.93004 -0.73075
H  -5.96914  3.94187 -0.51402
H  -4.39647  4.71562 -0.13327
H  -4.73965  4.20449 -1.78959
C  -6.29405 -0.64575  0.33755
H  -6.41519 -1.37342 -0.48448
H  -6.25776 -1.23424  1.26971
H  -7.17934  0.00721  0.36250
C  -2.17289  3.44954 -1.16577
C  -1.96706  3.49924 -2.57810
C  -1.11804  4.48965 -3.10489
H  -0.95670  4.53381 -4.18842
C  -0.47641  5.41705 -2.27741
H   0.18214  6.17942 -2.70804
C  -0.68427  5.36412 -0.89559
H  -0.18150  6.09169 -0.24828
C  -1.52858  4.39834 -0.31729
C  -2.64357  2.50909 -3.52931
H  -3.28332  1.85061 -2.91654
C  -3.55670  3.22047 -4.55175
H  -4.31849  3.84383 -4.05200
H  -2.97496  3.87650 -5.22472
H  -4.08207  2.47860 -5.18027
C  -1.60892  1.61744 -4.25050
H  -0.93757  2.22120 -4.88820
H  -0.98152  1.06390 -3.52992
H  -2.11832  0.88328 -4.90111
C  -1.72612  4.38266  1.19942
H  -2.53087  3.65905  1.41943
C  -0.45069  3.89870  1.92139
H  -0.16452  2.87859  1.60641
H   0.40611  4.56024  1.70266
H  -0.60372  3.87865  3.01447
C  -2.17470  5.75254  1.75183
H  -1.39023  6.52014  1.62346
H  -3.08561  6.11602  1.24467
H  -2.39114  5.67646  2.83258
C  -3.80480 -1.90918  0.22563
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C -3.73973 -2.69044 -0.96823
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C -3.56580 -4.72214 0.38403
H -3.47339 -5.81203 0.44602
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H -3.60058 -4.45144 2.52539
C -3.75557 -2.55129 1.50028
C -3.81503 -2.04908 -2.35595
H -3.95181 -0.96357 -2.20773
C -5.03108 -2.55964 -3.15980
H -4.94712 -3.64014 -3.37664
H -5.97560 -2.39967 -2.61122
H -5.10355 -2.02918 -4.12659
C -2.50841 -2.25479 -3.15262
H -1.63625 -1.83052 -2.62434
H -2.30453 -3.32756 -3.32011
H -2.57680 -1.76475 -4.14075
C -3.82497 -1.76167 2.80974
H -4.01978 -0.70636 2.55078
C -2.48137 -1.81621 3.56902
H -2.21444 -2.85514 3.83361
H -1.65639 -1.40538 2.95885
H -2.54627 -1.23385 4.50654
C -4.97396 -2.23803 3.72512
H -5.94753 -2.21118 3.20549
H -4.81028 -3.27314 4.07549
H -5.04546 -1.59138 4.61817
C -1.25129 1.50542 4.95590
H -0.72605 2.44527 5.21219
C   1.24719 -1.50445 4.95910
H   0.72158 -2.44430 5.21464
H   1.79818 -1.67664 4.01549
H   0.00016 -0.00017 1.34032
Zn -0.00201 0.00038 4.82191

II
SCF (TPSS/SVP) Energy = -5692.69696842
Enthalpy 298K = -5691.279244
Free Energy 298K = -5691.496446
Lowest Frequency = 4.0749 cm^{-1}
Second Frequency = 10.5099 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -5691.819989

Ca -1.67891 0.00073 0.72411
N -3.41587 1.57269 0.40981
N -3.41722 -1.56981 0.41035
C -4.62683 1.30073 0.92347
C -5.10587 0.00234 1.24700
H -6.09266 0.00285 1.71817
C -4.62772 -1.29662 0.92450
C -5.60048 2.44397 1.17623
H -6.51717 2.08845 1.67034
H -5.88008 2.93194 0.22638
H -5.13385 3.22487 1.80125
C -5.60184 -2.43909 1.17895
H -5.13513 -3.21969 1.80431
H -5.88243 -2.92777 0.22975
H -6.51795 -2.08264 1.67345
C -3.13629 2.89370 -0.06868
C -2.48044 3.84207 0.77179
C -2.14967 5.10600 0.24943
H -1.64231 5.83415 0.89273
C -2.46087 5.45409 -1.06828
H -2.20204 6.44595 -1.45513
C -3.10882 4.52284 -1.88637
H -3.35499 4.79529 -2.91956
C -3.45330 3.24219 -1.41635
C -2.12329 3.51496 2.22194
H -2.60029 2.55107 2.46793
C -2.66575 4.55989 3.21997
H -3.75605 4.69328 3.11044
H -2.19022 5.54696 3.07637
H -2.46226 4.24038 4.25792
C -0.59924 3.34253 2.39656
H -0.05789 4.27316 2.15123
H -0.19792 2.55887 1.72562

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C  -4.14950  2.26477 -2.36540
H  -4.32013  1.32914 -1.80673
C  -3.25647  1.92829 -3.57884
H  -2.30252  1.47604 -3.25957
H  -3.02248  2.83347 -4.16831
H  -3.76774  1.21572 -4.25018
C  -5.52355  2.79105 -2.83557
H  -5.41864  3.71425 -3.43447
H  -6.18660  3.01883 -1.98306
H  -6.02931  2.03813 -3.46718
C  -3.13892 -2.89132 -0.06749
C  -2.48223 -3.83921  0.77284
C  -2.15246 -5.10365  0.25109
H  -1.64443 -5.83140  0.89430
C  -2.46552 -5.45272 -1.06592
H  -2.20741 -6.44493 -1.45235
C  -3.11440 -4.52198 -1.88387
H  -3.36205 -4.79522 -2.91649
C  -3.45795 -3.24087 -1.41442
C  -2.12303 -3.51087  2.22218
H  -2.60015 -2.54703  2.46818
C  -2.66337 -4.55525  3.22191
H  -2.18755 -5.54220  3.07842
H  -3.75377 -4.68927  3.11415
H  -2.45842 -4.23476  4.25927
C  -0.59881 -3.33748  2.39424
H  -0.19901 -2.55412  1.72192
H  -0.05724 -4.26789  2.14855
H  -0.34712 -3.05838  3.43385
C  -4.15517 -2.26407 -2.36336
H  -4.32529 -1.32808 -1.80513
C  -3.26334 -1.92832 -3.57788
H  -3.02997 -2.83388 -4.16702
H  -2.30905 -1.47590 -3.25986
H  -3.77528 -1.21616 -4.24916
C  -5.52964 -2.79068 -2.83190
H  -6.19184 -3.01811 -1.97864
H  -5.42526 -3.71415 -3.43047
H  -6.03607 -2.03811 -3.46338
H  -0.12792  0.00003 -0.81561
Ca  1.93647 -0.00038 -0.20993
H   1.10010  0.84455  5.53588
H   2.41090  0.00534  4.66757
H  -2.08123 -0.87863  4.16415
N   3.58643 -1.52364 -0.89907
N   3.58728  1.52376 -0.89538
C   4.79125 -1.28741 -1.44343
C   5.32593  0.00047 -1.69037
H   6.32113  0.00074 -2.14300
C   4.79194  1.28806 -1.44042
C   5.67146 -2.46558 -1.83160
H   6.61976 -2.12873 -2.27658
H   5.89561 -3.09143 -0.95004
H   5.15168 -3.11980 -2.55303
C   5.67271  2.46661 -1.82617
H   5.15385  3.12166 -2.54754
H   5.89582  3.09149 -0.94369
H   6.62149  2.13019 -2.27046
C   3.15491 -2.87253 -0.68276
C   2.38574 -3.54306 -1.68135
C   1.86549 -4.81778 -1.39122
H   1.26259 -5.33458 -2.14636
C   2.10341 -5.43974 -0.16120
H   1.68901 -6.43303  0.04305
C   2.88019 -4.78805  0.80265
H   3.07653 -5.28379  1.76049
C   3.41826 -3.50922  0.56771
C   2.12966 -2.91570 -3.05376
H   2.72790 -1.98929 -3.10712
C   2.59621 -3.83257 -4.20555
H   3.65729 -4.11724 -4.09493
H   2.00183 -4.76302 -4.24986
H   2.47953 -3.31717 -5.17594
C   0.64713 -2.52537 -3.23559
H  -0.00977 -3.41135 -3.17272
H   0.31440 -1.81045 -2.46145
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H 0.48892 -2.05391 -4.22288
C 4.27161 -2.83712 1.64585
H 4.69781 -1.92034 1.20260
C 3.42179 -2.41385 2.86265
H 2.60851 -1.71970 2.58359
H 2.95170 -3.28958 3.34574
H 4.04544 -1.90551 3.61939
C 5.45262 -3.72497 2.09405
H 5.10289 -4.64186 2.60198
H 6.07611 -4.03337 1.23673
H 6.09565 -3.17627 2.80553
C 3.15637 2.87250 -0.67690
C 2.38868 3.54540 -1.67505
C 1.86920 4.82004 -1.38323
H 1.26743 5.33862 -2.13805
C 2.10647 5.43970 -0.15193
H 1.69275 6.43301 0.05361
C 2.88168 4.78565 0.81158
H 3.07750 5.27957 1.77047
C 3.41887 3.50676 0.57498
C 2.13313 2.92047 -3.04867
H 2.73161 1.99430 -3.10357
C 2.59957 3.83945 -4.19880
H 2.00480 4.76971 -4.24178
H 3.66051 4.12441 -4.08742
H 2.48338 3.32559 -5.17007
C 0.65074 2.53002 -3.23139
H 0.31804 1.81366 -2.45856
H -0.00642 3.41569 -3.16702
H 0.49279 2.06023 -4.21952
C 4.27086 2.83235 1.65276
H 4.69539 1.91507 1.20894
C 3.42039 2.41003 2.86946
H 2.95131 3.28631 3.35257
H 2.60647 1.71669 2.59029
H 4.04361 1.90110 3.62619
C 5.45350 3.71785 2.10141
H 6.07757 4.02549 1.24425
H 5.10537 4.63516 2.60968
H 6.09552 3.16769 2.81266
C 1.32749 -0.02154 4.88215
H 1.13593 -0.92860 5.49038
C -1.92747 0.00193 3.50762
H -2.07442 0.88256 4.16566
H -2.81931 0.00606 2.84228
H 0.61818 0.00090 1.63232
Zn 0.13061 -0.00481 3.29085

III

SCF (TPSS/SVP) Energy = -7551.61475798
Enthalpy 298K = -7550.118526
Free Energy 298K = -7550.349125
Lowest Frequency = 8.4865 cm^{-1}
Second Frequency = 13.2426 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -7550.731026

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H 1.49107 -3.85419 5.58644
H 2.68637 -1.51761 1.33236
N -3.66059 -1.67427 0.73452
N -3.43590 1.44369 1.24751
C -4.42874 -1.51414 1.81950
C -4.65857 -0.28579 2.49448
H -5.31934 -0.38512 3.36118
C -4.25753 1.04595 2.23821
C -5.14287 -2.70467 2.45646
H -4.62371 -2.99047 3.38942
H -5.16658 -3.58419 1.79604
H -6.17509 -2.43283 2.73314
C -4.82519 2.08519 3.19984
H -5.26002 2.94023 2.65597
H -4.02670 2.49905 3.84116
H -5.59634 1.64455 3.84961
C -3.55793 -2.95511 0.10310
C -4.35124 -3.22171 -1.05846
C -4.17407 -4.44211 -1.73519

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H  -4.77776 -4.65440 -2.62369
C  -3.25127 -5.39670 -1.29234
H  -3.13043 -6.34093 -1.83475
C  -2.49550 -5.13931 -0.14536
H  -1.78540 -5.89495  0.21092
C  -2.62998 -3.93461  0.57176
C  -5.42831 -2.23694 -1.52368
H  -5.10651 -1.23056 -1.20014
C  -6.78249 -2.52154 -0.83274
H  -6.70438 -2.45777  0.26372
H  -7.14605 -3.53317 -1.09062
H  -7.54329 -1.79017 -1.16176
C  -5.62345 -2.20796 -3.05208
H  -6.08911 -3.13918 -3.42314
H  -4.66934 -2.06588 -3.58646
H  -6.29608 -1.37669 -3.32877
C  -1.80534 -3.74135  1.84806
H  -2.05588 -2.74777  2.25841
C  -0.28987 -3.75557  1.56470
H  -0.00799 -2.95617  0.86107
H   0.04159 -4.72495  1.15216
H   0.27050 -3.58919  2.50647
C  -2.15149 -4.80356  2.91673
H  -1.85603 -5.81469  2.58232
H  -3.23100 -4.82746  3.13925
H  -1.60957 -4.59281  3.85696
C  -3.19231  2.84817  1.10205
C  -3.94241  3.60106  0.14765
C  -3.68577  4.97866  0.01613
H  -4.26828  5.56505 -0.70345
C  -2.70942  5.61622  0.78795
H  -2.52877  6.69067  0.67265
C  -1.96040  4.86933  1.70320
H  -1.18576  5.36785  2.29625
C  -2.18260  3.49167  1.88039
C  -5.03991  2.95339 -0.69997
H  -4.90368  1.85986 -0.61847
C  -6.45067  3.27368 -0.15589
H  -6.64151  4.36252 -0.17307
H  -6.57562  2.92307  0.88200
H  -7.22431  2.78279 -0.77427
C  -4.94355  3.34091 -2.19045
H  -3.93437  3.15411 -2.59565
H  -5.17854  4.40893 -2.34972
H  -5.66605  2.75367 -2.78512
C  -1.32848  2.71197  2.88303
H  -1.82130  1.73932  3.05300
C   0.07134  2.42137  2.29984
H   0.61566  3.35284  2.06891
H  -0.01969  1.83624  1.36425
H   0.67534  1.83005  3.01161
C  -1.20185  3.41669  4.24970
H  -2.19178  3.65929  4.67425
H  -0.62776  4.35747  4.17432
H  -0.67189  2.76472  4.96733
C   2.43346 -3.82221  5.00784
H   2.59207 -4.82532  4.56962
C   2.31559 -1.03855  2.26054
H   2.96555 -0.18553  2.52241
H   1.26352 -0.71616  2.12585
H  -0.20399 -0.57977  0.61177
Zn  2.36437 -2.45084  3.62365
Ca  1.64943  0.21452 -0.28880
H  -0.01494  0.52569 -5.33644
H   1.36241  1.05266 -4.32758
H  -3.53480  0.77007 -2.09655
N   3.16724  2.01253 -0.81437
N   3.25305 -1.07184 -1.47531
C   4.00692  1.96851 -1.85729
C   4.29124  0.81666 -2.64102
H   4.93451  1.02511 -3.50196
C   4.00022 -0.55511 -2.47006
C   4.76287  3.21429 -2.31338
H   4.35483  3.56404 -3.27863
H   4.69177  4.03926 -1.58949
H   5.82619  2.97394 -2.48124
C   4.57701 -1.47505 -3.54151
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H   3.82873 -1.61184 -4.34474
H   5.47892 -1.03950 -3.99940
C   3.00184  3.22839 -0.07594
C   3.66734  3.36511  1.18163
C   3.45871  4.53033  1.94118
H   3.97377  4.64621  2.90080
C   2.61137  5.54946  1.49132
H   2.46289  6.45122  2.09564
C   1.96003  5.40782  0.26235
H   1.29804  6.20729 -0.08975
C   2.13570  4.26460 -0.54127
C   4.64133  2.29179  1.67150
H   4.34159  1.34407  1.18659
C   6.08494  2.59176  1.20703
H   6.14810  2.66911  0.10967
H   6.44142  3.54582  1.63664
H   6.77346  1.79033  1.53277
C   4.60579  2.08151  3.19784
H   5.03041  2.94477  3.74142
H   3.57619  1.92789  3.56595
H   5.20784  1.19726  3.47423
C   1.40815  4.18942 -1.88635
H   1.67093  3.22779 -2.35858
C  -0.12521  4.21786 -1.71606
H  -0.47361  3.41767 -1.04243
H  -0.46897  5.17924 -1.29592
H  -0.61813  4.08570 -2.69660
C   1.84370  5.32464 -2.84134
H   1.52984  6.31147 -2.45443
H   2.93691  5.35243 -2.98017
H   1.37429  5.18968 -3.83245
C   3.21916 -2.48699 -1.27103
C   4.13935 -3.07993 -0.34790
C   4.03200 -4.45605 -0.07657
H   4.73399 -4.92237  0.62337
C   3.05062 -5.24710 -0.68668
H   2.98362 -6.31629 -0.45739
C   2.16549 -4.66433 -1.59827
H   1.40595 -5.28747 -2.08437
C   2.23484 -3.29391 -1.91353
C   5.25321 -2.24977  0.29916
H   4.90681 -1.20009  0.30273
C   6.55456 -2.29489 -0.53584
H   6.93287 -3.33065 -0.61364
H   6.39785 -1.91161 -1.55604
H   7.33908 -1.67836 -0.06004
C   5.56521 -2.65740  1.75266
H   4.65527 -2.66841  2.37965
H   6.02714 -3.65910  1.81356
H   6.27564 -1.94180  2.20371
C   1.27184 -2.70719 -2.94716
H   1.60119 -1.67412 -3.15492
C  -0.17254 -2.63041 -2.41063
H  -0.57266 -3.62971 -2.16473
H  -0.22381 -2.02637 -1.48277
H  -0.84013 -2.17487 -3.16376
C   1.30674 -3.47819 -4.28433
H   2.33428 -3.55365 -4.67970
H   0.91244 -4.50431 -4.17181
H   0.68414 -2.96266 -5.03723
C   0.27533  1.18203 -4.49226
H   0.12639  2.22499 -4.83925
C  -2.79280  0.18132 -2.68016
H  -3.15804  0.24775 -3.72113
H  -2.93862 -0.88879 -2.41025
H  -0.20199  0.93769 -1.28333
Zn -0.83228  0.82050 -2.87801
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TS(III-IV)

SCF (TPSS/SVP) Energy = -7551.61354749
Enthalpy 298K = -7550.118259
Free Energy 298K = -7550.345168
Lowest Frequency = -15.6726 cm^{-1}
Second Frequency = 10.5367 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -7550.7311

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H  -0.84079 -2.32700  5.53611
H   2.13299 -1.64211  1.75757
N  -3.69815 -1.33183  0.67878
N  -3.24115  1.76463  1.06160
C  -4.44906 -1.07602  1.75729
C  -4.57295  0.18855  2.39253
H  -5.23379  0.17413  3.26480
C  -4.08785  1.47740  2.06831
C  -5.26294 -2.18302  2.42353
H  -4.75823 -2.50395  3.35314
H  -5.37746 -3.06566  1.77658
H  -6.26130 -1.81267  2.70953
C  -4.59055  2.60160  2.96863
H  -4.91371  3.47548  2.37926
H  -3.78316  2.95488  3.63509
H  -5.42855  2.26217  3.59618
C  -3.72279 -2.62143  0.05796
C  -4.52810 -2.80917 -1.11114
C  -4.45941 -4.03825 -1.79143
H  -5.07143 -4.19016 -2.68652
C  -3.63264 -5.07586 -1.34478
H  -3.59307 -6.02432 -1.89183
C  -2.87115 -4.89626 -0.18687
H  -2.24002 -5.71690  0.17409
C  -2.90161 -3.68768  0.53593
C  -5.50339 -1.72443 -1.57841
H  -5.08030 -0.75365 -1.26226
C  -6.87490 -1.86827 -0.87794
H  -6.78357 -1.80875  0.21778
H  -7.34073 -2.83879 -1.12924
H  -7.55997 -1.06473 -1.20515
C  -5.70403 -1.68394 -3.10554
H  -6.25973 -2.56743 -3.46945
H  -4.74373 -1.63632 -3.64540
H  -6.29532 -0.79295 -3.38250
C  -2.09069 -3.58342  1.83085
H  -2.26342 -2.57695  2.24998
C  -0.57534 -3.72754  1.58607
H  -0.20477 -2.94610  0.90327
H  -0.31854 -4.71512  1.16430
H  -0.02771 -3.62748  2.54403
C  -2.55750 -4.62387  2.87535
H  -2.33576 -5.65249  2.53732
H  -3.64228 -4.56068  3.06223
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H  -3.80772  5.72221 -1.27816
C  -2.26213  5.82452  0.22395
H  -2.00934  6.86719  0.00206
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H  -0.77973  5.63729  1.78115
C  -1.88856  3.79389  1.53633
C  -4.75337  3.17760 -1.01571
H  -4.64223  2.08632 -0.88048
C  -6.14003  3.55957 -0.44915
H  -6.30196  4.65149 -0.51062
H  -6.24589  3.25817  0.60590
H  -6.94246  3.06272 -1.02470
C  -4.69420  3.48395 -2.52631
H  -3.69767  3.26764 -2.94780
H  -4.92819  4.54307 -2.73796
H  -5.43639  2.87077 -3.06805
C  -1.10330  3.07511  2.63582
H  -1.64655  2.14553  2.87816
C   0.30006  2.66965  2.13806
H   0.89027  3.54683  1.82326
H   0.21998  1.98370  1.27288
H   0.85835  2.14821  2.93644
C  -0.98984  3.90349  3.93310
H  -1.98048  4.23218  4.29281
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H  -0.51730  3.30208  4.73068
C   0.24763 -2.50768  5.61755
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H   1.68421  0.01325  2.37235
H  -0.13989 -0.54543  0.69657
Zn  1.20283 -1.75277  4.09449
Ca  1.78659 -0.01170 -0.24542
H   0.30514  0.22160 -5.33749
H   1.69334  0.68364 -4.31369
H  -3.25939  0.98164 -2.21228
N   3.51445  1.56420 -0.79030
N   3.24457 -1.55711 -1.28183
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C   4.60335  0.11779 -2.45183
H   5.33083  0.18870 -3.26648
C   4.13146 -1.19650 -2.23000
C   5.31011  2.47266 -2.26778
H   4.97400  2.80662 -3.26592
H   5.30931  3.34346 -1.59587
H   6.34401  2.10628 -2.38155
C   4.68553 -2.25115 -3.18230
H   4.88098 -3.20692 -2.67033
H   3.94609 -2.45898 -3.97780
H   5.61118 -1.90354 -3.66619
C   3.45403  2.84016 -0.14158
C   4.08227  2.99269  1.13377
C   3.98097  4.22699  1.80041
H   4.46905  4.35459  2.77247
C   3.27579  5.29966  1.24275
H   3.21161  6.25495  1.77540
C   2.65633  5.14119 -0.00030
H   2.10416  5.98182 -0.43615
C   2.72693  3.92843 -0.71334
C   4.90609  1.85562  1.74219
H   4.50856  0.91281  1.32250
C   6.38872  1.94516  1.31345
H   6.49517  1.92216  0.21717
H   6.84379  2.88331  1.68045
H   6.96533  1.09840  1.72919
C   4.80218  1.77577  3.27747
H   5.30281  2.62995  3.76817
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H   5.29692  0.85830  3.64398
C   2.03838  3.83511 -2.07755
H   2.19833  2.81534 -2.46686
C   0.51483  4.05750 -1.97081
H   0.05059  3.35417 -1.25985
H   0.27697  5.08062 -1.62998
H   0.04044  3.91570 -2.95888
C   2.63750  4.83295 -3.09519
H   2.43448  5.87711 -2.79426
H   3.72974  4.71946 -3.19157
H   2.18613  4.67816 -4.09171
C   2.99031 -2.94819 -1.05689
C   3.70667 -3.62961 -0.02330
C   3.41130 -4.98267  0.22490
H   3.95949 -5.51699  1.00813
C   2.43464 -5.66444 -0.51034
H   2.22199 -6.71841 -0.29997
C   1.73426 -4.99040 -1.51490
H   0.96876 -5.52513 -2.08862
C   1.99571 -3.63923 -1.80980
C   4.80291 -2.92095  0.77753
H   4.55629 -1.84355  0.76635
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H   6.47611 -4.13511  0.03595
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H   6.96215 -2.55350  0.71603
C   4.87864 -3.38281  2.24663
H   3.88953 -3.36333  2.73553
H   5.27733 -4.40992  2.33344
H   5.55776 -2.72337  2.81639
C   1.20413 -2.94229 -2.91721
H   1.69979 -1.97806 -3.12386
C  -0.23615 -2.62827 -2.46142
H  -0.80059 -3.54766 -2.22562
H  -0.23836 -2.00770 -1.54255
```

H -0.78391 -2.08632 -3.25321
C   1.18457 -3.74183 -4.23685
H   2.20572 -3.99468 -4.57099
H   0.62021 -4.68619 -4.13417
H   0.69844 -3.14934 -5.03223
C   0.62651 0.89618 -4.51926
H   0.57828 1.92697 -4.92565
C -2.57382 0.29052 -2.74954
H -2.91090 0.34307 -3.80082
H -2.83656 -0.74403 -2.43318
H   0.04199 0.83509 -1.31836
Zn -0.55680 0.71574 -2.92818

IV
SCF (TPSS/SVP) Energy = -7551.63904289
Enthalpy 298K = -7550.142456
Free Energy 298K = -7550.369827
Lowest Frequency = 7.3145 cm^{-1}
Second Frequency = 9.5852 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -7550.755938

Ca -1.98405 0.13700 -0.07218
H -0.71315 0.45125 4.94683
H -2.04831 -0.09591 3.89624
H   2.97842 -1.02361 2.19134
N -3.74683 -1.25120 0.73927
N -3.29106 1.86659 0.85516
C -4.58334 -0.88715 1.72073
C -4.72799 0.43024 2.23197
H -5.44206 0.49963 3.05825
C -4.19692 1.67924 1.83473
C -5.47651 -1.91540 2.40880
H -5.06978 -2.14069 3.41137
H -5.54203 -2.85834 1.84596
H -6.49158 -1.51067 2.55526
C -4.70531 2.87884 2.62628
H -4.89996 3.74624 1.97528
H -3.94176 3.19677 3.35973
H -5.62325 2.62908 3.17978
C -3.75180 -2.59266 0.23420
C -4.47952 -2.87639 -0.96533
C -4.40071 -4.16816 -1.51652
H -4.95640 -4.39450 -2.43252
C -3.63651 -5.17425 -0.91409
H -3.59022 -6.17386 -1.36021
C -2.94454 -4.89573 0.26779
H -2.36011 -5.68899 0.74844
C -2.98624 -3.62054 0.86488
C -5.38902 -1.82412 -1.60683
H -4.98710 -0.83440 -1.32345
C -6.82523 -1.90762 -1.03886
H -6.84183 -1.76992 0.05362
H -7.27671 -2.89102 -1.26494
H -7.46369 -1.12587 -1.48962
C -5.43370 -1.89991 -3.14561
H -5.96354 -2.80432 -3.49600
H -4.42313 -1.90456 -3.58762
H -5.97847 -1.02791 -3.54928
C -2.24923 -3.40195 2.18914
H -2.38965 -2.34769 2.48183
C -0.73148 -3.65119 2.07051
H -0.27253 -3.00997 1.29945
H -0.50739 -4.69903 1.80395
H -0.23533 -3.44209 3.03600
C -2.83132 -4.28865 3.31445
H -2.64445 -5.35924 3.11244
H -3.91993 -4.15417 3.42317
H -2.35535 -4.04132 4.28047
C -2.94398 3.20551 0.47926
C -3.60741 3.81927 -0.62817
C -3.22446 5.11786 -1.01158
H -3.73403 5.59931 -1.85340
C -2.21197 5.81044 -0.33868
H -1.93169 6.82153 -0.65397
C -1.56173 5.20159 0.73891
H -0.76669 5.74368 1.26346
C -1.91007 3.90751 1.16809

```
C  -4.74626  3.11270 -1.36815
H  -4.65599  2.03526 -1.13974
C  -6.13165  3.56640 -0.85295
H  -6.27189  4.65180 -1.00916
H  -6.25556  3.35804  0.22218
H  -6.93655  3.03685 -1.39483
C  -4.66896  3.28804 -2.89881
H  -3.67111  3.02702 -3.29074
H  -4.89013  4.32718 -3.20291
H  -5.41287  2.63800 -3.39326
C  -1.16928  3.28267  2.35142
H  -1.71892  2.37246  2.64615
C   0.25573  2.84732  1.95047
H   0.87587  3.70507  1.63670
H   0.22849  2.14189  1.09548
H   0.76417  2.35294  2.79805
C  -1.11252  4.20951  3.58395
H  -2.11964  4.55217  3.87802
H  -0.49458  5.10538  3.39338
H  -0.66702  3.67477  4.44166
C  -1.00934 -0.31749  4.20565
H  -1.03123 -1.28381  4.74861
C   2.35998 -0.22382  2.65416
H   2.62065 -0.26848  3.72691
H   2.77656  0.75145  2.31647
H  -0.17256 -0.52171  1.04564
Zn  0.30017 -0.38683  2.71076
Ca  1.98411 -0.13712  0.07212
H   0.71349 -0.45235 -4.94648
H   2.04825  0.09675 -3.89641
H  -2.97905  1.02227 -2.19173
N   3.74682  1.25144 -0.73896
N   3.29175 -1.86679 -0.85434
C   4.58389  0.88720 -1.71988
C   4.72913 -0.43032 -2.23061
H   5.44367 -0.49976 -3.05648
C   4.19805 -1.67936 -1.83348
C   5.47718  1.91540 -2.40789
H   5.07101  2.14011 -3.41081
H   5.54213  2.85862 -1.84545
H   6.49245  1.51087 -2.55355
C   4.70696 -2.87890 -2.62480
H   4.90060 -3.74657 -1.97387
H   3.94412 -3.19632 -3.35922
H   5.62559 -2.62926 -3.17721
C   3.75124  2.59317 -0.23458
C   4.47853  2.87774  0.96503
C   4.39943  4.16985  1.51536
H   4.95481  4.39683  2.43140
C   3.63536  5.17549  0.91203
H   3.58889  6.17540  1.35747
C   2.94374  4.89613 -0.26984
H   2.35937  5.68902 -0.75118
C   2.98570  3.62055 -0.86608
C   5.38791  1.82598  1.60753
H   4.98646  0.83604  1.32429
C   6.82447  1.90965  1.04048
H   6.84181  1.77150 -0.05194
H   7.27553  2.89326  1.26644
H   7.46285  1.12826  1.49197
C   5.43152  1.90243  3.14631
H   5.96090  2.80712  3.49669
H   4.42065  1.90704  3.58763
H   5.97623  1.03073  3.55074
C   2.24892  3.40103 -2.19031
H   2.38933  2.34656 -2.48222
C   0.73116  3.65046 -2.07209
H   0.27205  3.00990 -1.30058
H   0.50710  4.69853 -1.80640
H   0.23515  3.44065 -3.03750
C   2.83120  4.28689 -3.31619
H   2.64437  5.35764 -3.11496
H   3.91980  4.15227 -3.42470
H   2.35531  4.03890 -4.28208
C   2.94444 -3.20575 -0.47875
C   3.60739 -3.81973  0.62884
C   3.22414 -5.11831  1.01197
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H 3.73335 -5.59993 1.85391
C 2.21181 -5.81070 0.33862
H 1.93128 -6.82178 0.65371
C 1.56211 -5.20168 -0.73920
H 0.76725 -5.74364 -1.26416
C 1.91080 -3.90761 -1.16812
C 4.74611 -3.11345 1.36931
H 4.65616 -2.03598 1.14097
C 6.13159 -3.56742 0.85461
H 6.27156 -4.65285 1.01082
H 6.25596 -3.35903 -0.22046
H 6.93640 -3.03807 1.39682
C 4.66819 -3.28892 2.89993
H 3.67026 -3.02771 3.29151
H 4.88901 -4.32815 3.20400
H 5.41208 -2.63912 3.39472
C 1.17083 -3.28272 -2.35194
H 1.72081 -2.37260 -2.64632
C -0.25442 -2.84702 -1.95220
H -0.87532 -3.70464 -1.63957
H -0.22780 -2.14200 -1.09685
H -0.76153 -2.35194 -2.80018
C 1.11483 -4.20961 -3.58448
H 2.12212 -4.55235 -3.87785
H 0.49670 -5.10541 -3.39427
H 0.66995 -3.67486 -4.44251
C 1.00905 0.31720 -4.20589
H 1.03007 1.28312 -4.74960
C -2.36018 0.22249 -2.65398
H -2.62099 0.26610 -3.72674
H -2.77598 -0.75282 -2.31542
H 0.17258 0.52147 -1.04588
Zn -0.30042 0.38652 -2.71092

TS(IV-V)
SCF (TPSS/SVP) Energy = -7551.63737194
Enthalpy 298K = -7550.141814
Free Energy 298K = -7550.364712
Lowest Frequency = -38.8980 cm^{-1}
Second Frequency = 7.9292 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -7550.752196

Ca -2.04924 -0.12134 -0.13273
H -1.01153 -0.62916 -4.41141
H -2.24701 -0.03773 -3.27528
H 3.01393 0.69570 -2.12157
N -3.93458 1.18128 -0.77643
N -3.39711 -1.91150 -0.86061
C -4.77907 0.78617 -1.73965
C -4.88899 -0.53910 -2.24033
H -5.61437 -0.63949 -3.05346
C -4.34136 -1.77184 -1.81000
C -5.71637 1.78535 -2.41061
H -5.29764 2.07311 -3.39252
H -5.84433 2.70150 -1.81476
H -6.70408 1.33352 -2.59792
C -4.88602 -3.00774 -2.51621
H -5.07223 -3.83034 -1.80662
H -4.14835 -3.38164 -3.24946
H -5.81740 -2.77936 -3.05624
C -4.02778 2.49601 -0.21076
C -4.77088 2.67080 1.00028
C -4.77548 3.93491 1.61647
H -5.34269 4.07728 2.54230
C -4.07610 5.01698 1.06957
H -4.09164 5.99273 1.56758
C -3.36870 4.84401 -0.12287
H -2.83645 5.69647 -0.56098
C -3.33163 3.60145 -0.78579
C -5.59971 1.52681 1.59081
H -5.13113 0.58561 1.25159
C -7.04450 1.54063 1.03910
H -7.06465 1.46345 -0.05938
H -7.56126 2.47552 1.32389
H -7.62190 0.69183 1.44937
C -5.63109 1.51634 3.13152
H -6.20590 2.36898 3.53669

H	-4.61616	1.55127	3.56104
H	-6.12321	0.59484	3.49105
C	-2.58894	3.50024	-2.12051
H	-2.67008	2.45624	-2.46790
C	-1.08848	3.83406	-1.98825
H	-0.58721	3.17225	-1.26278
H	-0.93195	4.87616	-1.65707
H	-0.58331	3.71853	-2.96481
C	-3.23289	4.40725	-3.19479
H	-3.11711	5.47504	-2.93361
H	-4.31078	4.20667	-3.31053
H	-2.74543	4.24771	-4.17374
C	-3.05070	-3.22512	-0.40182
C	-3.66681	-3.73500	0.78284
C	-3.28225	-5.00301	1.25583
H	-3.75618	-5.40400	2.15843
C	-2.31155	-5.76484	0.59675
H	-2.02710	-6.75004	0.98235
C	-1.70824	-5.25772	-0.55787
H	-0.94639	-5.85440	-1.07249
C	-2.06057	-3.99835	-1.07795
C	-4.75804	-2.94943	1.51364
H	-4.65884	-1.89579	1.19572
C	-6.17205	-3.41319	1.09466
H	-6.32589	-4.47864	1.34640
H	-6.33567	-3.29217	0.01133
H	-6.94431	-2.82292	1.62128
C	-4.61436	-3.00358	3.04827
H	-3.59666	-2.72657	3.37280
H	-4.83275	-4.01170	3.44476
H	-5.32766	-2.30541	3.52170
C	-1.36506	-3.48901	-2.34155
H	-1.90730	-2.59038	-2.68091
C	0.08728	-3.06174	-2.04506
H	0.69627	-3.90974	-1.68442
H	0.12170	-2.28504	-1.25553
H	0.56833	-2.65435	-2.95173
C	-1.39460	-4.51346	-3.49562
H	-2.42325	-4.84973	-3.71310
H	-0.79123	-5.40914	-3.26213
H	-0.97782	-4.06426	-4.41485
C	-1.23966	0.17481	-3.68516
H	-1.33315	1.11401	-4.26697
C	2.26972	-0.04310	-2.48986
H	2.44925	-0.09167	-3.57915
H	2.58340	-1.04407	-2.11835
H	-0.08506	0.88857	-0.77536
Zn	0.26492	0.37699	-2.38949
Ca	2.04908	0.12161	0.13295
H	1.01224	0.63053	4.41106
H	2.24722	0.03837	3.27478
H	-3.01423	-0.69385	2.12229
N	3.93407	-1.18163	0.77638
N	3.39771	1.91138	0.86051
C	4.77885	-0.78676	1.73945
C	4.88924	0.53848	2.24010
H	5.61475	0.63864	3.05314
C	4.34195	1.77140	1.80985
C	5.71598	-1.78620	2.41025
H	5.29741	-2.07376	3.39229
H	5.84349	-2.70243	1.81443
H	6.70388	-1.33468	2.59728
C	4.88685	3.00704	2.51636
H	5.07075	3.83073	1.80746
H	4.15029	3.37914	3.25166
H	5.81954	2.77893	3.05426
C	4.02669	-2.49645	0.21080
C	4.76930	-2.67158	-1.00049
C	4.77330	-3.93574	-1.61656
H	5.34012	-4.07836	-2.54260
C	4.07383	-5.01757	-1.06930
H	4.08890	-5.99336	-1.56722
C	3.36694	-4.84428	0.12340
H	2.83462	-5.69655	0.56180
C	3.33046	-3.60165	0.78621
C	5.59830	-1.52790	-1.59138
H	5.12998	-0.58652	-1.25232

C 7.04316 -1.54191 -1.03984
H 7.06345 -1.46445 0.05861
H 7.55968 -2.47698 -1.32446
H 7.62069 -0.69333 -1.45040
C 5.62951 -1.51778 -3.13210
H 6.20417 -2.37058 -3.53715
H 4.61454 -1.55267 -3.56151
H 6.12171 -0.59642 -3.49189
C 2.58823 -3.50010 2.12116
H 2.66988 -2.45612 2.46848
C 1.08760 -3.83335 1.98936
H 0.58641 -3.17143 1.26394
H 0.93058 -4.87543 1.65834
H 0.58275 -3.71750 2.96604
C 3.23215 -4.40732 3.19528
H 3.11588 -5.47508 2.93418
H 4.31016 -4.20716 3.31071
H 2.74504 -4.24755 4.17437
C 3.05165 3.22502 0.40156
C 3.66801 3.73459 -0.78311
C 3.28365 5.00253 -1.25645
H 3.75774 5.40327 -2.15906
C 2.31293 5.76462 -0.59767
H 2.02862 6.74975 -0.98354
C 1.70948 5.25786 0.55703
H 0.94768 5.85476 1.07147
C 2.06160 3.99856 1.07744
C 4.75941 2.94880 -1.51343
H 4.65965 1.89512 -1.19578
C 6.17331 3.41199 -1.09344
H 6.32766 4.47744 -1.34488
H 6.33618 3.29072 -0.01003
H 6.94570 2.82155 -1.61967
C 4.61675 3.00329 -3.04814
H 3.59914 2.72680 -3.37339
H 4.83588 4.01137 -3.44431
H 5.33004 2.30487 -3.52122
C 1.36605 3.48973 2.34123
H 1.90783 2.59080 2.68053
C -0.08664 3.06336 2.04515
H -0.69518 3.91174 1.68466
H -0.12178 2.28665 1.25567
H -0.56770 2.65632 2.95197
C 1.39656 4.51429 3.49517
H 2.42550 4.84991 3.71234
H 0.79375 5.41035 3.26170
H 0.97971 4.06550 4.41456
C 1.23988 -0.17370 3.68493
H 1.33315 -1.11281 4.26693
C -2.26976 0.04492 2.49012
H -2.44912 0.09402 3.57942
H -2.58323 1.04580 2.11819
H 0.08469 -0.88806 0.77575
Zn -0.26510 -0.37573 2.38969

v
SCF (TPSS/SVP) Energy = -7551.66671230
Enthalpy 298K = -7550.170189
Free Energy 298K = -7550.397279
Lowest Frequency = 6.1102 cm^{-1}
Second Frequency = 10.9173 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -7550.762655

Ca -0.73207 2.26986 -1.33126
H -1.49075 3.06955 1.02389
H -2.70154 1.98505 0.27369
H -0.45925 -1.15385 3.31610
N -2.30437 3.34400 -2.72353
N 0.31448 4.37198 -1.29433
C -2.58549 4.64578 -2.51812
C -1.74353 5.57440 -1.85635
H -2.16629 6.58222 -1.79441
C -0.38887 5.50344 -1.42186
C -3.89460 5.21111 -3.05443
H -4.75190 4.64173 -2.65520
H -3.94397 5.11640 -4.15259
H -4.01488 6.27159 -2.78626

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C   0.24254  6.85612 -1.10882
H   1.33597  6.78679 -1.00670
H  -0.16749  7.25397 -0.16270
H  -0.00038  7.58521 -1.89977
C  -3.07897  2.60816 -3.68168
C  -2.70689  2.65255 -5.06175
C  -3.43276  1.88443 -5.98963
H  -3.15155  1.92192 -7.04867
C  -4.49842  1.07022 -5.59301
H  -5.04856  0.47757 -6.33209
C  -4.85022  1.01980 -4.24190
H  -5.68374  0.38111 -3.92674
C  -4.16498  1.77795 -3.27322
C  -1.53500  3.50127 -5.56166
H  -1.05133  3.94643 -4.67590
C  -2.00136  4.65861 -6.47267
H  -2.72261  5.31736 -5.95984
H  -2.48769  4.27522 -7.38847
H  -1.13959  5.27734 -6.78308
C  -0.48070  2.64022 -6.29110
H  -0.89314  2.19153 -7.21303
H  -0.12013  1.81843 -5.64960
H   0.38636  3.25956 -6.58435
C  -4.61242  1.68055 -1.81458
H  -4.00981  2.40813 -1.24132
C  -4.34685  0.27318 -1.23446
H  -3.28187 -0.01108 -1.30558
H  -4.92811 -0.49430 -1.77656
H  -4.63563  0.22540 -0.16917
C  -6.09433  2.07098 -1.62518
H  -6.76781  1.36097 -2.13837
H  -6.30263  3.07852 -2.02520
H  -6.35908  2.06627 -0.55237
C   1.70112  4.37307 -0.93504
C   2.66869  4.10455 -1.95141
C   4.02631  4.01681 -1.59601
H   4.77224  3.82078 -2.37356
C   4.44405  4.17839 -0.27093
H   5.50625  4.10603 -0.01295
C   3.49239  4.43130  0.72034
H   3.81969  4.55342  1.75940
C   2.12052  4.53188  0.42035
C   2.25280  3.96728 -3.41634
H   1.18201  3.69167 -3.42266
C   2.36646  5.32343 -4.14958
H   3.41527  5.67236 -4.16274
H   1.75802  6.09943 -3.65513
H   2.02178  5.23329 -5.19602
C   3.03057  2.87075 -4.16983
H   2.98834  1.90524 -3.63589
H   4.09467  3.13793 -4.30129
H   2.60416  2.72517 -5.17757
C   1.13965  4.79372  1.56547
H   0.12983  4.88361  1.12875
C   1.11379  3.61540  2.56328
H   2.09776  3.48100  3.04758
H   0.85564  2.66844  2.05993
H   0.36674  3.79544  3.35754
C   1.44815  6.11310  2.30806
H   1.48144  6.97312  1.61836
H   2.42251  6.06137  2.82679
H   0.67547  6.31341  3.07233
C  -1.87774  2.02637  1.01760
H  -2.39088  1.91650  1.99051
C   0.11430 -0.28241  2.92649
H  -0.14479  0.53837  3.61962
H   1.19025 -0.47875  3.12876
H  -0.82618 -0.92839  0.04878
Zn -0.48968  0.49628  1.11172
Ca  0.73207 -2.26986  1.33126
H   1.49075 -3.06955 -1.02389
H   2.70154 -1.98505 -0.27369
H   0.45925  1.15385 -3.31610
N   2.30437 -3.34400  2.72353
N  -0.31448 -4.37198  1.29433
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H   3.94397 -5.11640  4.15259
H   4.01488 -6.27159  2.78626
C  -0.24254 -6.85612  1.10882
H  -1.33597 -6.78679  1.00670
H   0.16749 -7.25397  0.16270
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C   2.70689 -2.65255  5.06175
C   3.43276 -1.88443  5.98963
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H   0.89314 -2.19153  7.21303
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H  -3.81969 -4.55342 -1.75940
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C  -2.25280 -3.96728  3.41634
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H  -1.48144 -6.97312 -1.61836
H  -2.42251 -6.06137 -2.82679
H  -0.67547 -6.31341 -3.07233
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H   0.14479 -0.53837 -3.61962
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Zn  0.48968 -0.49628 -1.11172
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4
SCF (TPSS/SVP) Energy = -3912.32782619
Enthalpy 298K = -3910.928183
Free Energy 298K = -3911.135794
Lowest Frequency = 8.3864 cm^{-1}
Second Frequency = 17.3662 cm^{-1}
SCF (PBE0-D3(C6H6)/def2-TZVPP) Energy = -3911.455657

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C	-4.53046	1.25809	1.51468
C	-3.17307	-2.90871	0.25095
C	-4.94158	-0.05119	1.88084
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C	-3.19348	2.90506	0.40299
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H	-4.00246	5.05311	-2.15079
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H	-4.87833	-3.05774	2.74733
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C	-6.10030	3.12452	-1.88914
H	-6.58963	3.40491	-0.94061
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H   1.24912 -0.67483  2.12059
```

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