Supporting Information

Fluorenyl-Tethered N-Heterocyclic Carbene (NHC): An Exclusive C-donor Ligand for Heteroleptic Calcium and Strontium Chemistry.

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Table of Contents

1. **General procedures.**

All reactions were performed under a dry argon atmosphere using standard Schlenk techniques or under argon atmosphere in a glovebox, unless otherwise indicated. Prior to use, glassware were dried overnight at 130 °C and solvents were dried, distilled and degassed using standard methods. The imidazolium salt precursor [(L*H*)(X*H*)]Br and the potassium complex $[(LX)K]_n$ were made by following the reported procedure.[1] KHMDS, CaI_2, SrI_2 and were purchased from Sigma and used as received inside the glovebox. The aminoalkenes were made following standard literature procedure and purified by drying and distilling over CaH_2 and stored in the glovebox with molecular sieves prior to uses.[2] ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded on a Bruker Avance NEO (500 MHz) or Avance III (500 MHz) spectrometer at ambient temperature unless otherwise mentioned. Chemical shifts (δ ppm) in the ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were referenced to the residual signals of the deuterated solvents. Abbreviations for NMR spectra: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), sept (septet), br (broad). Elemental analyses were performed on a PerkinElmer series II 2400 machine. X-ray diffraction data for compounds **1-4•THF** were collected on a Rigaku Synergy i diffractometer. Single crystal diffraction data are reported in crystallographic information files (cif) accompanying this document.

2. **Experimental Procedure and Spectroscopic data.**

[(LX)CaI(thf)$_2$] (1).

A 1 ml THF solution of $[(LX)K]_n$ (0.100 g, 0.218 mmol) was added dropwise to another 1 mL THF suspension of finely grounded CaI_2 (0.064 g, 0.218 mmol). The reaction was stirred for 3 h. The resulting greenish yellow solution was then filtered through celite, and the volatiles were removed under reduced pressure. The greenish yellow residue was washed with benzene (3 × 2 mL) and dried under vacuum to obtain [(LX)CaI(thf)$_2$] (**1**, 0.131 g, 0.179 mmol, 82%) as a greenish yellow powder. Elemental analysis for $C_{38}H_{47}N_2O_2ICa$: Calcd. C, 62.46; H, 6.48; N, 3.83; Found C, 62.12; H, 6.55; N, 3.62.

[(LX)SrI(thf)$_2$] (2).

Following a similar protocol, $[(LX)K]_n$ (0.100 g, 0.218 mmol) and SrI_2 (0.074 g, 0.218 mmol) afforded [LSrI(thf)$_2$] (**2**, 0.142 g, 0.183 mmol, 84%) as a greenish yellow powder. Elemental analysis for $C_{38}H_{47}N_2O_2ISr$: Calcd. C, 58.64; H, 6.09; N, 3.60; Found C, 58.06; H, 6.30; N, 3.49.

The NMR spectra of both **1** and **2** are overly broad and not reported herein.

[(LX)Ca{N(SiMe$_3$)$_2$}(thf)] (3•THF).

A 1 mL toluene solution of [Ca{N(SiMe$_3$)$_2$}$_2$(thf)$_2$] (0.505 g, 1.000 mmol) was added dropwise to another 1 mL toluene suspension of [(L*H*)X*H*]Br (0.501 g, 1.000 mmol). The reaction was stirred for 1 h. After complete dissolution of the insoluble [(L*H*)X*H*]Br, a 1 mL THF solution of KN(SiMe$_3$)$_2$ (0.200 g, 1.000 mmol) was added dropwise and stirred for 3 h. The reaction mixture was then filtered and the filtrate was concentrated to dryness under reduced pressure. Washing the residue with hexane (3 × 5 mL) followed by drying under vacuum gave **3•THF** (0.625 g, 0.903 mmol, 90%) as a golden yellow powder. It was however crystallized as the THF-free reddish-colored **3**, though in poor yield, as confirmed by X-ray crystallography. The poor yield allowed us only to record the ^{1}H NMR spectrum of **3** and to perform a hydroamination catalysis of 1-amino-2,2-diphenylpent-4-ene.

^{1}H NMR (500 MHz, C_6D_6) δ 8.35 (d, *J* = 8.1 Hz, 2 H, Ar*H*), 7.40 – 7.33 (m, 4 H, Ar*H*), 7.14 – 7.12 (m, 2 H, Ar*H*), 7.06 – 7.02 (m, 1 H, Ar*H*), 6.89 (d, *J* = 7.8 Hz, 2 H, Ar*H*), 6.23 (d, *J* = 1.6 Hz, 1 H, NC*H*), 6.18 (d, *J* = 1.6 Hz, 1 H, NC*H*), 3.89 – 3.85 (m, 2 H, CH_2), 3.51 (br, 4 H, thf), 3.16 – 3.12 (m, 2 H, CH_2), 2.19 (sep, *J* = 6.8 Hz, 2 H, C*H*(CH$_3$)$_2$), 1.40 – 1.35 (m, 4 H, thf), 1.09 (d, *J* = 6.8 Hz, 6 H, CH(CH_3)$_2$), 0.87 (d, *J* = 6.9 Hz, 6 H, CH(CH_3)$_2$), 0.30 (tms), 0.10 (N(Si*Me*$_3$)$_2$), -0.23 (s, 18 H, [Ca{N(SiMe$_3$)}]). ^{13}C{1H} NMR (126 MHz, 5:1 C_6D_6/THF-d_8) δ 194.9 (NCN), 146.1 (Ar, *C*), 137.4 (Ar, *C*), 133.4 (Ar, *C*), 129.6 (Ar, *C*), 124.2 (Ar, *C*), 124 (Ar, *C*), 123.1 (Ar, *C*), 122.9 (Ar, *C*), 121.6 (Ar, *C*), 119.1 (Ar, *C*), 116.1 (Ar, *C*), 115.5 (Ar, *C*), 91.2 (fluorenyl-*C*), 67.8 (thf), 67 (p, thf-d_8), 53.7 (*C*H$_2$), 28.6 (*C*H$_2$), 28.1 (*C*H(CH$_3$)$_2$), 25.9 (CH(*C*H$_3$)$_2$), 25.8 (thf), 24.7 (p, thf-d_8), 23.6 (CH(*C*H$_3$)$_2$), 5.9 (Ca{N(Si*Me*$_3$)}), 2.6 (N(Si*Me*$_3$)$_2$), 1.4 (tms). Elemental analysis for $C_{40}H_{57}N_3OSi_2Ca$: Calcd. C, 69.41; H, 8.30; N, 6.07; Found C, 68.90; H, 8.39; N, 6.17.

3:

^{1}H NMR (400 MHz, C_6D_6) δ 8.35 (dt, *J* = 8.2, 1.0 Hz, 2H), 7.44 – 7.29 (m, 4H), 7.15 – 7.11 (m, 2H), 7.06 – 7.02 (m, 1H), 6.90 (d, *J* = 7.7 Hz, 2H), 6.22 (d, *J* = 1.6 Hz, 1H), 6.17 (d, *J* = 1.6 Hz, 1H), 3.86 – 3.84 (m, 2H), 3.15 – 3.12 (m, 2H), 2.22 – 2.09 (p, *J* = 6.8 Hz, 2H), 1.09 (d, *J* = 6.9 Hz, 6H), 0.87 (d, *J* = 6.8 Hz, 6H), -0.25 (s, 18H).

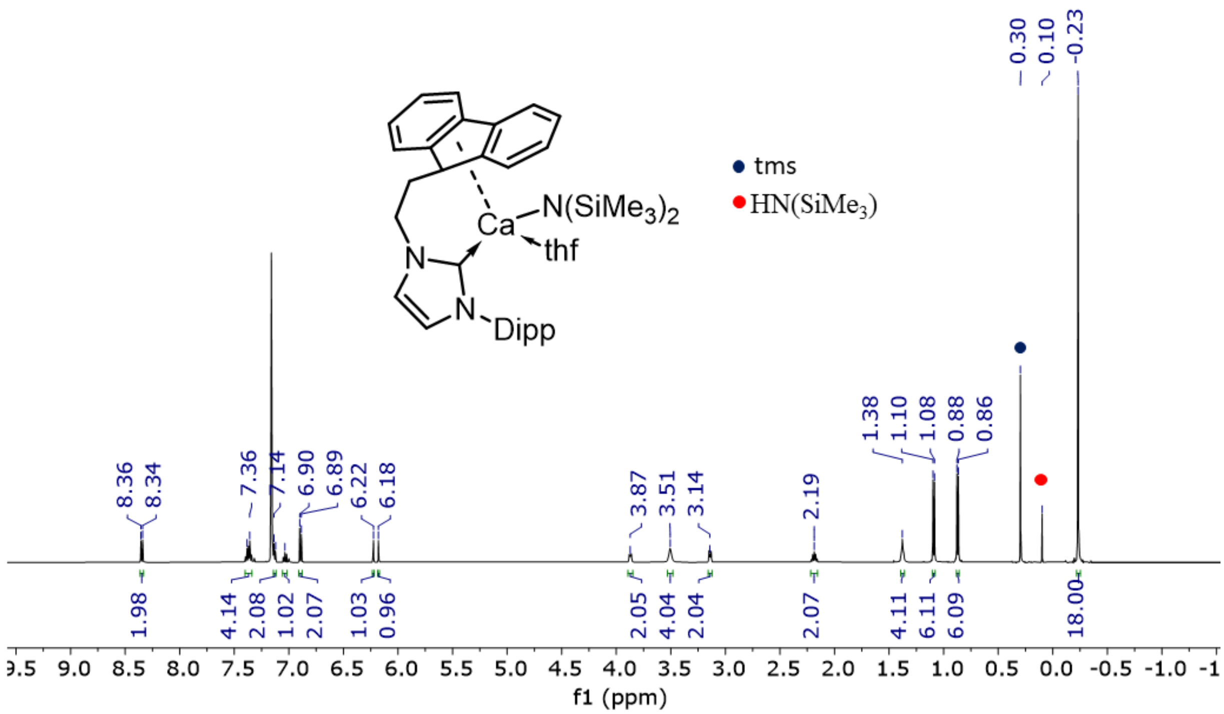


Figure S1. ^{1}H NMR spectrum of **3•THF** in C_6D_6.

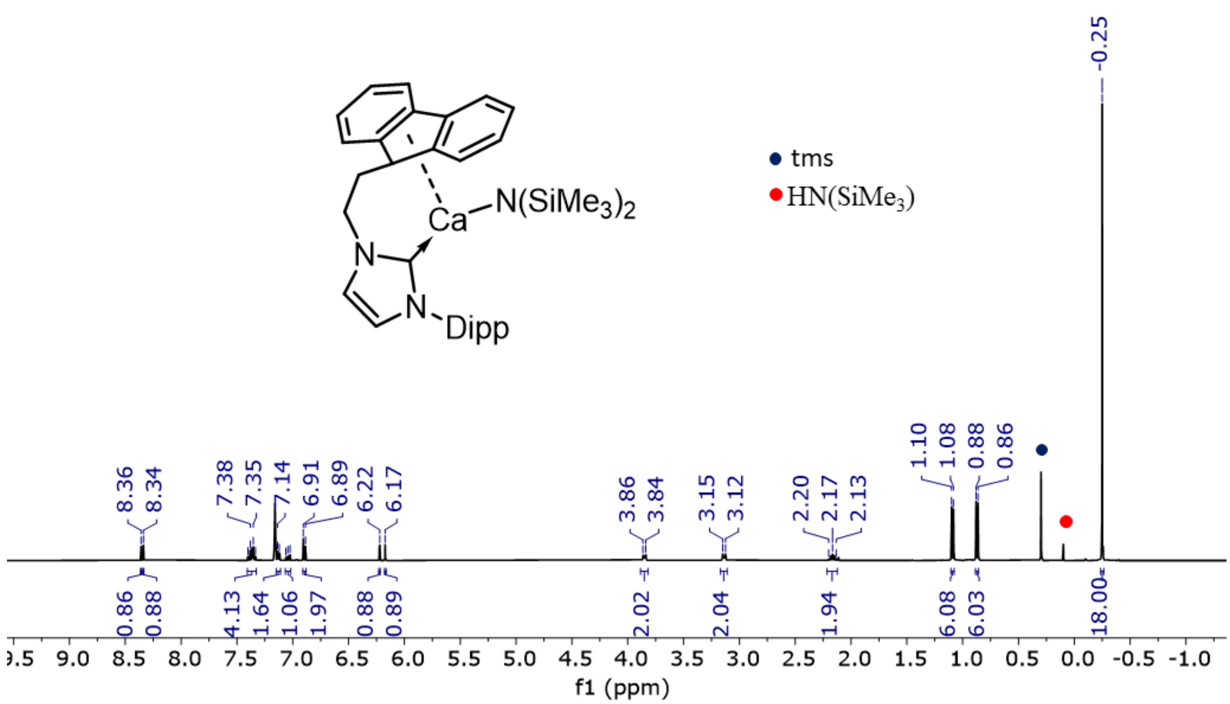


Figure S2. ^{1}H NMR spectrum of **3** in C_6D_6.

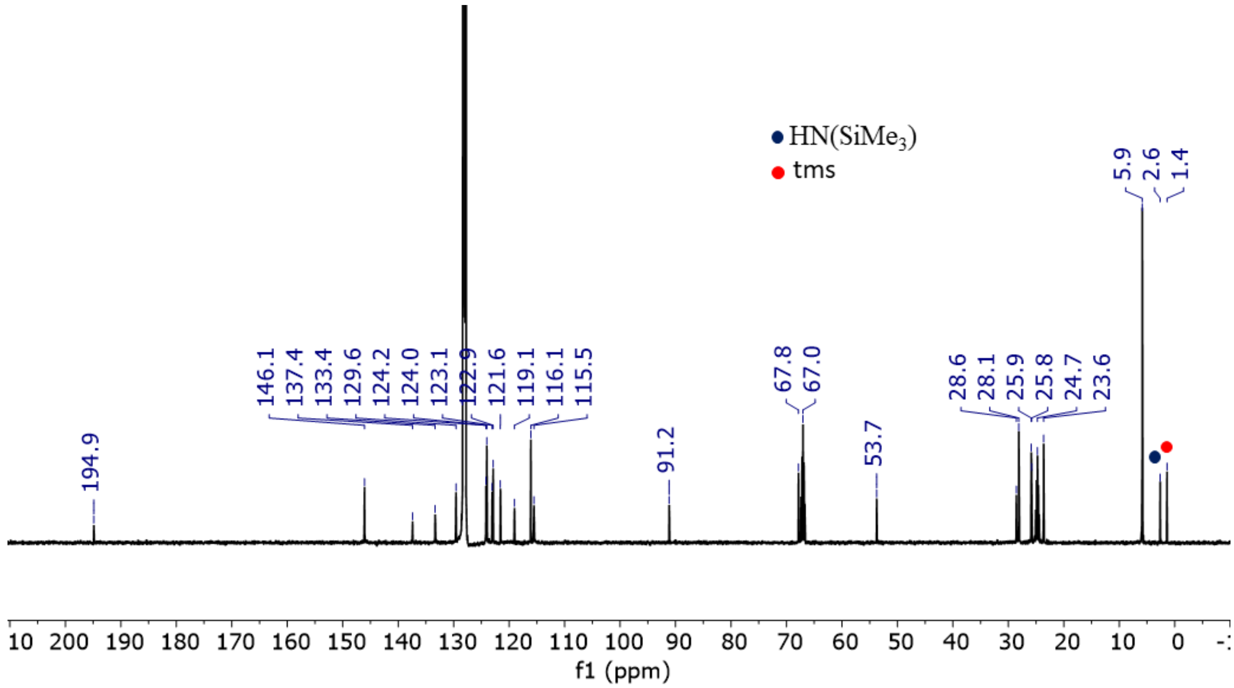


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of **3•THF** in 5:1 C_6D_6/THF-d_8 mixture.

[(LX)Sr{N(SiMe$_3$)$_2$}(thf)] (4•THF).

A 1 ml THF solution of [(LX)K]$_n$ (0.100 g, 0.218 mmol) was added dropwise to another 1 mL THF suspension of finely grounded SrI_2 (0.074 g, 0.218 mmol) and KN(SiMe$_3$)$_2$ (0.044 g, 0.220 mmol). The reaction was stirred for 4 h. The resulting yellow ochre-colored solution was then filtered through celite and concentrated to dryness to obtain a yellow ochre residue. The residue was washed with hexane (3 × 2 mL) and dried under vacuum to obtain **4•THF** (0.145 g, 0.196 mmol, 90%) as a yellow ochre powder.

^{1}H NMR (500 MHz, 5:1 C_6D_6/THF-d_8) δ 8.33 (d, *J* = 8.0 Hz, 2 H, Ar*H*), 7.42 – 7.32 (m, 4 H, Ar*H*), 7.07 (br, 2 H, Ar*H*), 6.97 (t, *J* = 7.7 Hz, 1 H, Ar*H*), 6.86 (d, *J* = 7.8 Hz, 2 H, Ar*H*), 6.48 (s, 1 H, NC*H*), 6.40 (s, 1 H, NC*H*), 4.24 (br, 2 H, C*H*$_2$), 3.54 (m, 4 H, thf), 3.51 (br, thf-d_8), 3.29 (br, 2 H, C*H*$_2$), 2.48 (sept, *J* = 7.0 Hz, 2 H, C*H*(CH$_3$)$_2$), 1.44 (m, 4 H, thf), 1.40 (br, thf-d$_8$) 1.07 (d, *J* = 6.9 Hz, 6 H, CH(C*H*$_3$)$_2$), 0.90 (d, *J* = 6.8 Hz, 6 H, CH(C*H*$_3$)$_2$), 0.30 (tms), 0.24 ([Sr{N(SiMe$_3$)}$_2$]), 0.08 (N(Si*Me*$_3$)$_2$), 0.02 (s, 18 H, [Sr{N(SiMe$_3$)}]). $^{13}C\{^{1}H\}$ NMR (126 MHz, 5:1 C_6D_6/THF-d_8) δ 199.1 (N*C*N), 146.1 (Ar, *C*), 137.4 (Ar, *C*), 133.7 (Ar, *C*), 129.4 (Ar, *C*), 124.0 (Ar, *C*), 123.8 (Ar, *C*), 122.8 (Ar, *C*), 122.2 (Ar, *C*), 121.6 (Ar, *C*), 118.9 (Ar, *C*), 115.5 (Ar, *C*), 114.7 (Ar, *C*), 92.1 (fluorenyl-*C*), 67.8 (thf), 67.0 (p, thf-d_8), 53.8 (*C*H$_2$), 28.7 (*C*H$_2$), 28.1 (*C*H(CH$_3$)$_2$), 25.8 (thf), 24.8 (p, thf-d_8), 23.9 (CH(*C*H$_3$)$_2$), 5.8 [Sr{N(SiMe$_3$)}], 2.6 (N(Si*Me*$_3$)$_2$), 1.4 (tms). Elemental analysis for $C_{40}H_{57}N_3OSi_2Sr$: Calcd. C, 64.95; H, 7.77; N, 5.68; Found C, 64.41; H, 7.66; N, 5.80.

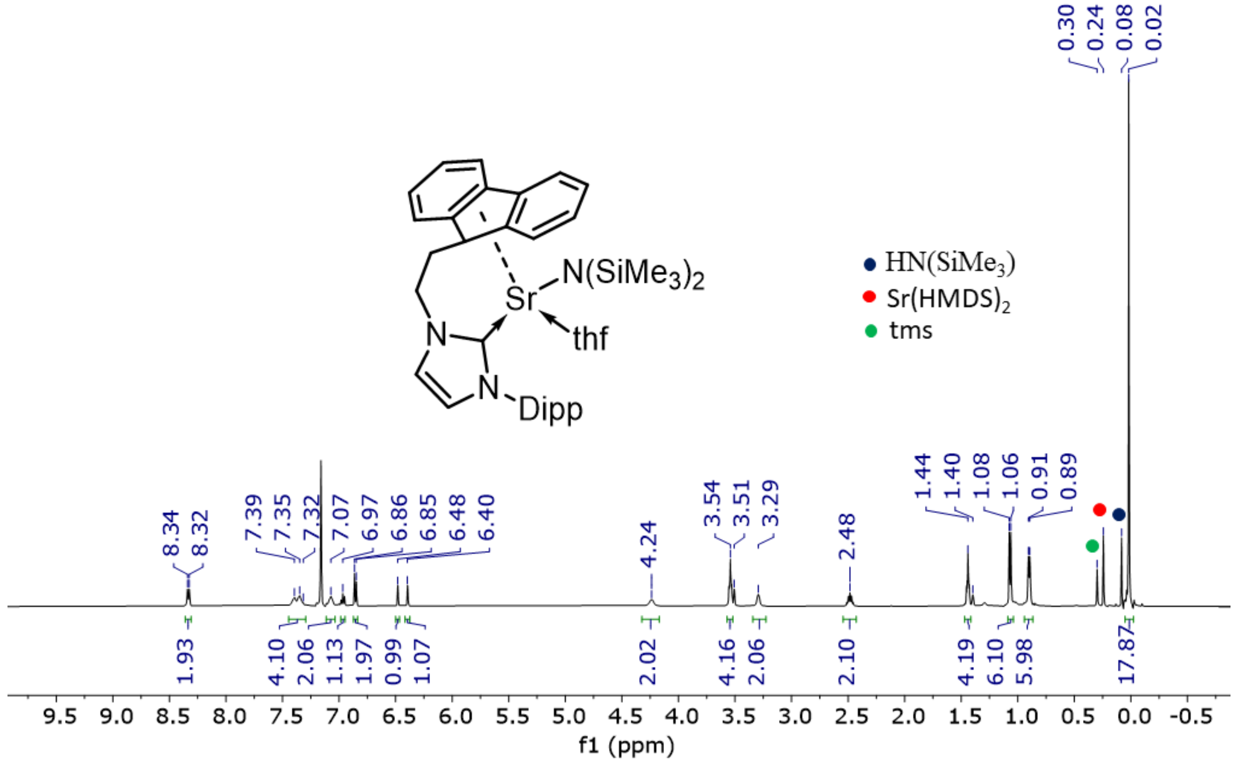


Figure S4. ^{1}H NMR spectrum of **4** in 5:1 C_6D_6/THF-d_8.

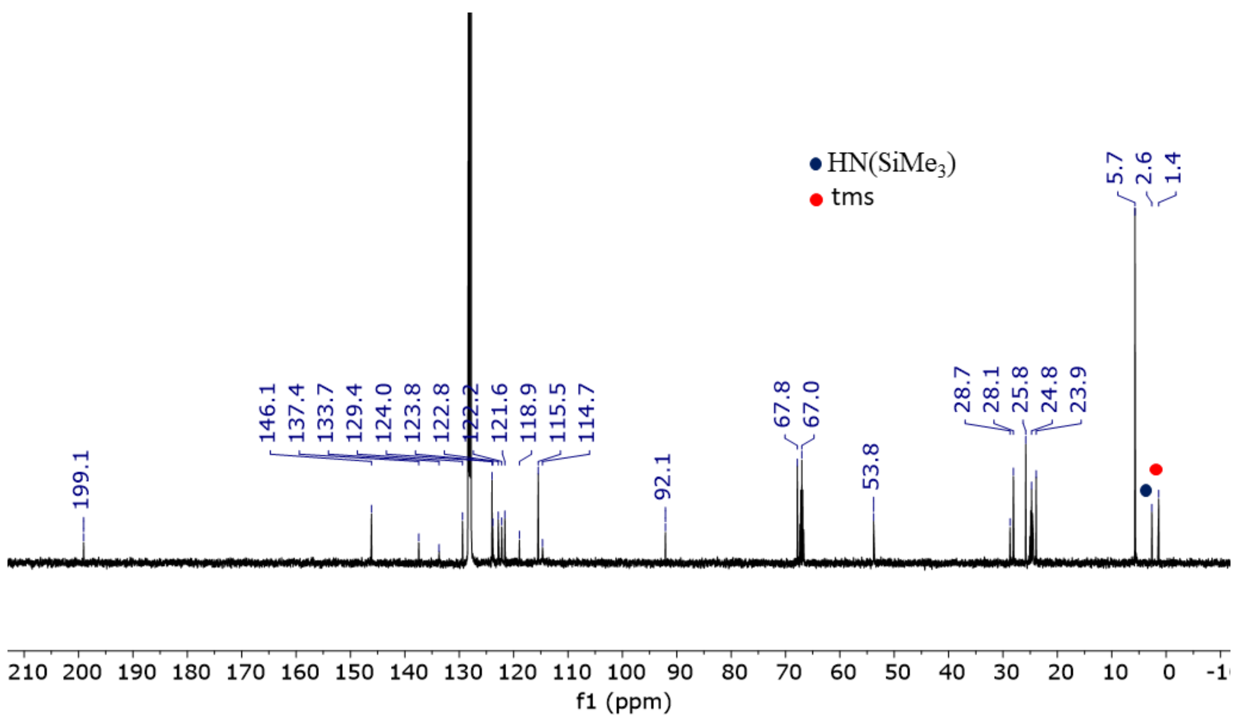


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in 5:1 C_6D_6/THF-d_8.

General procedure for the intramolecular hydroamination with catalyst 3•THF.

A 0.4 mL benzene solution mixture of aminoalkenes (0.250 mmol), and 1,3,5-trimethoxybenzene (0.021 g, 0.125 mmol, as an internal standard) was added to 0.4 mL suspension of the precatalyst **3•THF** (0.025 mmol). The resulting mixture was allowed to stir and the reaction progress was monitored from time to time by taking aliquots and analyzing by ^{1}H NMR spectrum in $CDCl_3$. Notably, the THF-free **3** appears to be nearly three times more efficient than **3•THF**, as tested for the hydroamination catalysis of 1-amino-2,2-diphenylpent-4-ene. A negative solvent effect is also observed with THF compared to benzene. The hydroamination catalysis of 1-amino-2,2-diphenylpent-4-ene by 10 mol% of **3•THF** in THF is slow, giving only 50% conversion after 1 h. In comparison, the same catalysis in benzene goes to completion within 30 min.

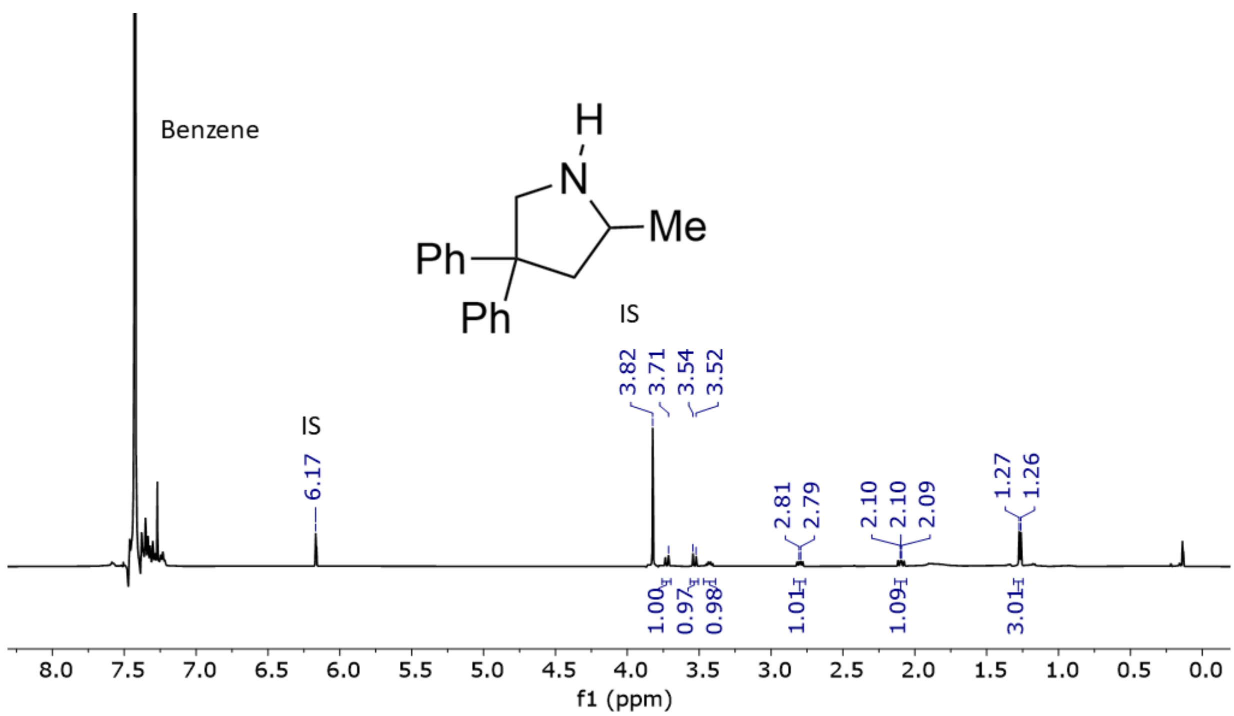


Figure S6. ^{1}H NMR spectrum of the reaction mixture of 1-amino-2,2-diphenylpent-4-ene hydroamination catalyzed by **3•THF** in $CDCl_3$.

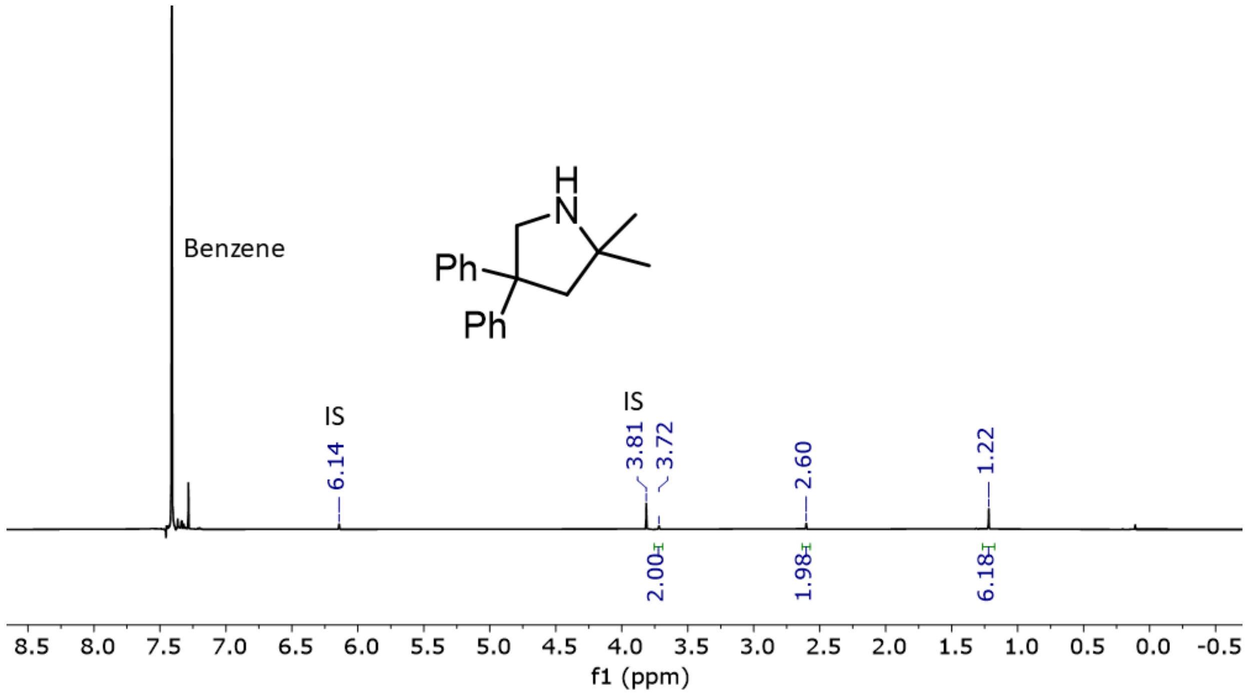


Figure S7. ^{1}H NMR spectrum of the reaction mixture of 1-amino-2,2-diphenyl-4-methylpent-4-ene hydroamination catalyzed by **3•THF** in $CDCl_3$.

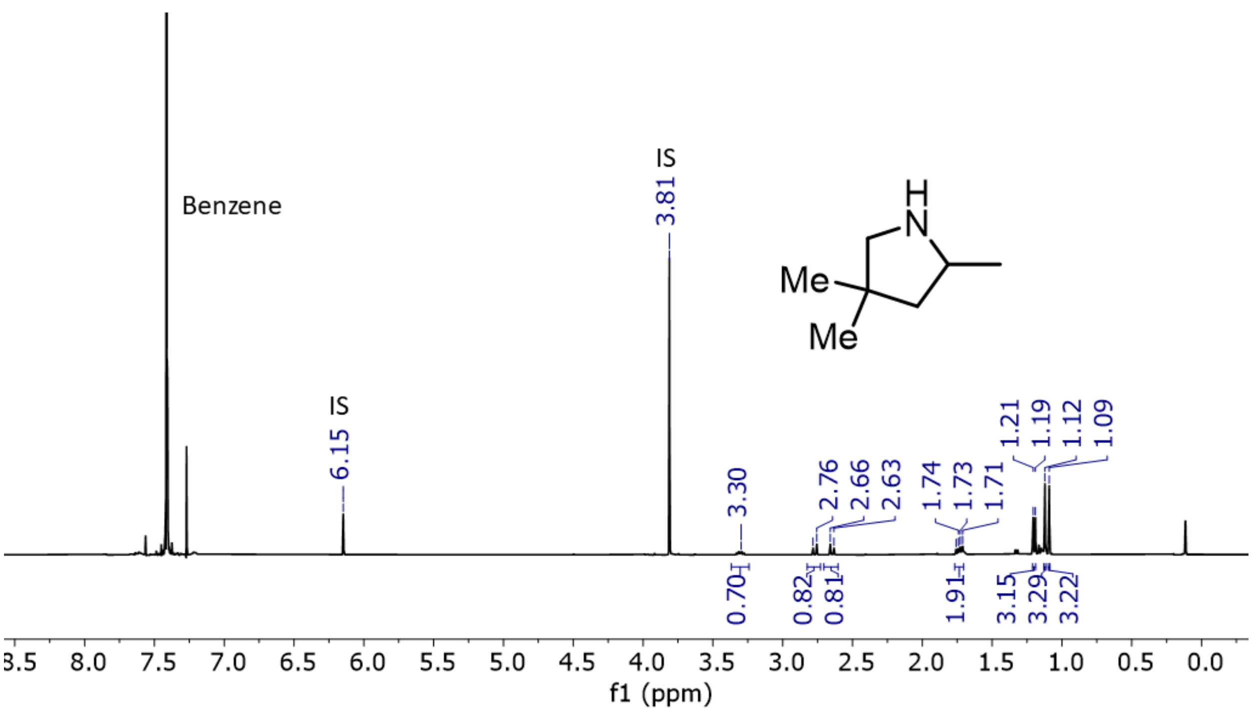


Figure S8. ^{1}H NMR spectrum of the reaction mixture of 1-amino-2,2-dimethylpent-4-ene hydroamination catalyzed by **3•THF** in $CDCl_3$.

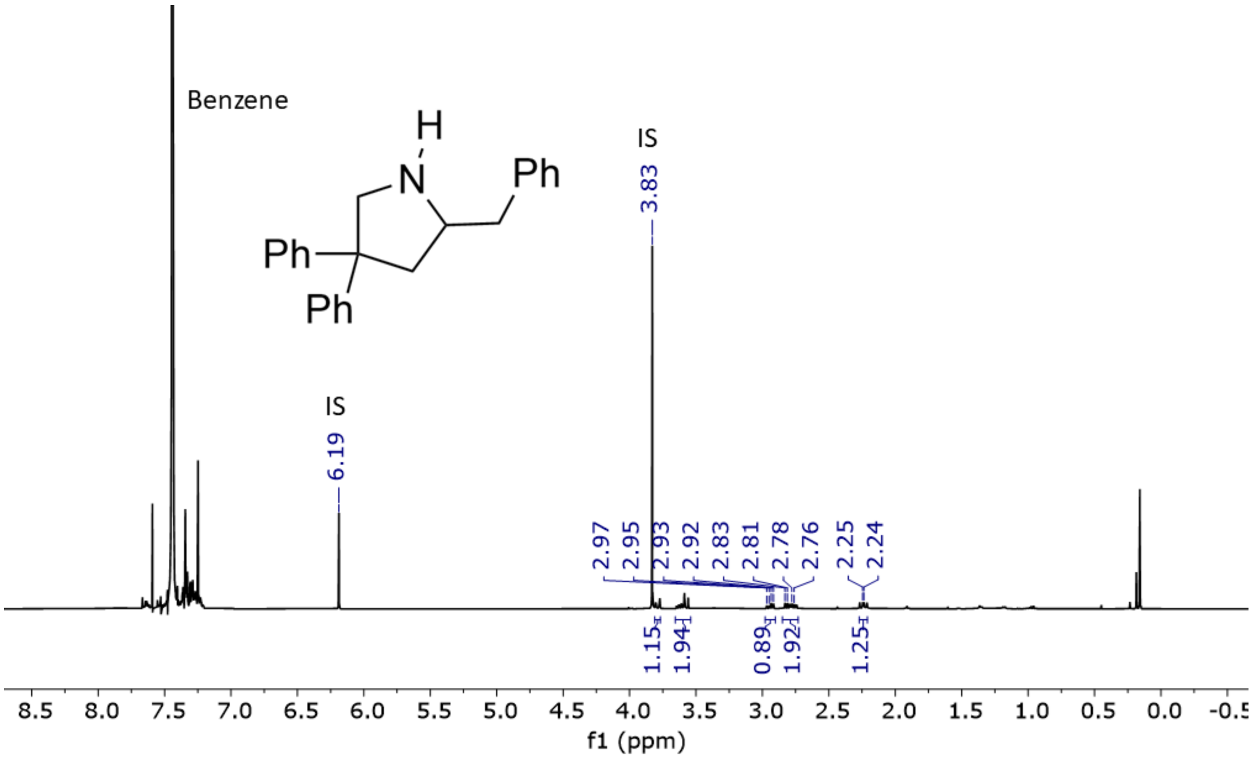


Figure S9. ^{1}H NMR spectrum of the reaction mixture of (2,2,5-triphenylpent-4-enyl) amine hydroamination catalyzed by **3•THF** in $CDCl_3$.

3. Crystallographic Data.

X-ray diffraction data were collected on a Rigaku XtaLAB Synergy, Dualflex four-circle diffractometer with HyPix3000 detector and Cu-K_{α} radiation. Measurements were carried out at 100 K **[(LX)CaI(thf)$_2$] (1)**, **[(LX)SrI(thf)$_2$] (2), [(LX)Ca{N(SiMe$_3$)$_2$}] (3)**, and **[(LX)Sr{N(SiMe$_3$)$_2$}(thf)] (4)**. The structures were solved by intrinsic phasing using SHELXT.[3] All refinements were carried out against F^2 with ShelXL[4] as implemented in the program system Olex2.[5] The non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were included in calculated positions and treated as riding throughout the refinement. [**(LX)CaI(thf)$_2$] (1)**, **[(LX)SrI(thf)$_2$] (2), [(LX)Ca{N(SiMe$_3$)$_2$}] (3)**, and **[(LX)Sr{N(SiMe$_3$)$_2$}(thf)] (4)** all of them having solvent related disorder. Refinement results are given in Table S1. Graphical representations were performed with the program DIAMOND.[6] CCDC- 2326768 **[(LX)CaI(thf)$_2$]** (**1**), CCDC- 2326769 **[(LX)SrI(thf)$_2$]** (**2**), CCDC- 2326770 **[(LX)Ca{N(SiMe$_3$)$_2$}]** (**3**), and CCDC- 2326771 **[(LX)Sr{N(SiMe$_3$)$_2$}(thf)]** (**4•THF**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1: Crystallographic data of **[(LX)CaI(thf)$_2$]** (**1**), and **[(LX)SrI(thf)$_2$]** (**2**).

	[(LX)CaI(thf)$_2$] (1)	**[(LX)SrI(thf)$_2$] (2)**
formula	$C_{44}H_{53}CaIN_2O_2$	$C_{44}H_{53}IN_2O_2Sr$
Fw /g·mol^{-1}	808.86	856.40
cryst. color, habit	Greenish yellow	Greenish yellow
Crystal size/ mm^3	0.38 × 0.19 × 0.13	0.6 × 0.29 × 0.21
crystal system	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$
a / Å	11.14530 (10)	11.13660(10)
b / Å	21.64110 (10)	21.95800(10)
c / Å	16.45190 (10)	16.44100(10)
α / °	90	90
β / °	99.6200 (10)	99.2670(10)
γ / °	90	90
V / Å^3	3912.34 (5)	3967.97 (5)
Z	4	4
d_{calc}/Mg·m^{-3}	1.373	1.434
μ(CuKα)/mm^{-1}	7.867	8.281
F(000)	1680.0	1752.0
2θ range / °	6.81 to 136.656	6.774 to 136.094
index ranges	$-13 \leq h \leq 13$, $-25 \leq k \leq 22$, $-19 \leq l \leq 19$	$-11 \leq h \leq 13$, $-26 \leq k \leq 26$, $-19 \leq l \leq 19$
refln.	46269	48895
independ. reflns (R_{int})	7115 [R_{int} = 0.0542, R_{sigma} = 0.0274]	7006 [R_{int} = 0.0775, R_{sigma} = 0.0367]
observed reflns	6752	6693
data/ restr./ param.	7115/0/455	7006/32/465
$R1$, $wR2$ [$I > 2\sigma(I)$]	R_1 = 0.0234, wR_2 = 0.0597	R_1 = 0.0418, wR_2 = 0.1104
$R1$, $wR2$ (all data)	R_1 = 0.0247, wR_2 = 0.0604	R_1 = 0.0430, wR_2 = 0.1215
GooF on F^2	1.061	1.087
largest diff. peak, hole/ e·Å^3	0.45/-0.58	2.41/-1.05
CCDC number	2326768	2326769

Table S2: Crystallographic data of **[(LX)Ca{N(SiMe$_3$)$_2$}] (3)**, and **[(LX)Sr{N(SiMe$_3$)$_2$}(thf)] (4•THF).**

	[(LX)Ca{N(SiMe$_3$)$_2$}] (3)	**[(LX)Sr{N(SiMe$_3$)$_2$}(thf)] (4•THF)**
formula	$C_{35.99}H_{48.98}CaN_3Si_2$	$C_{40}H_{57}N_3OSi_2Sr$
Fw /g·mol^{-1}	619.94	739.68
cryst. color, habit	Dark red	Greenish yellow
Crystal size/ mm^3	0.349 × 0.302 × 0.104	0.4 × 0.22 × 0.1
crystal system	monoclinic	monoclinic
space group	C2/c	C2/c
a / Å	21.9451 (2)	22.9542 (3)
b / Å	9.60320 (10)	9.94500 (10)
c / Å	35.7576 (3)	37.2321 (4)
α / °	90	90
β / °	105.8930(10)	105.9360 (10)
γ / °	90	90
V / Å^3	7247.62 (12)	8172.69 (17)
Z	8	8
d_{calc}/Mg·m^{-3}	1.136	1.202
μ(CuKα)/mm^{-1}	2.321	2.633
F(000)	2672.0	3136.0
2θ range / °	5.14 to 136.358	8.012 to 133.198
index ranges	$-26 \leq h \leq 25$, $-11 \leq k \leq 11$, $-40 \leq l \leq 43$	$-27 \leq h \leq 26$, $0 \leq k \leq 11$, $0 \leq l \leq 44$
refln.	27194	7203
independ. reflns (R_{int})	6555 [R_{int} = 0.0286, R_{sigma} = 0.0195]	7203 [R_{int} = MERG, R_{sigma} = 0.0341]
observed reflns	6373	6833
data/ restr./ param.	6559/0/394	7203/9/439
*R*1, *wR*2 [*I*> 2σ(*I*)]	R_1 = 0.0394, wR_2 = 0.1002	R_1 = 0.0568, wR_2 = 0.1786
*R*1, *wR*2 (all data)	R_1 = 0.0401, wR_2 = 0.1007	R_1 = 0.0588, wR_2 = 0.1803
GooF on F^2	1.042	1.057
largest diff. peak, hole/ e·Å^3	0.30/-0.44	0.73/-0.52
CCDC number	2326770	2326771

4. DFT analyses

DFT calculations were carried out using the Gaussian 16[7] program. The structures of all the complexes were optimised using the B3LYP[8] functional in the gas phase with Grimme's D3[9] parameter set with Becke-Johnson (BJ) damping.[10] The 6-311G** basis set[11] was used to describe C, H, N, O and Si atoms while the def2-TZVP basis set[12] was used for Ca, Sr and I atoms (pseudopotentials were applied for Sr and I). This combination is referred to as the B3LYP-D3/B1 level of theory. The vibrational frequencies were calculated at this level to characterise the stationary points as minima and to obtain zero-point vibrational energies. Single-point energy calculations were performed using the def2TZVP basis set for all atoms i.e. B3LYP-D3/B2 level of theory. Topological analysis was performed to evaluate electron density (ρ), Laplacian of electron density ($\nabla^2\rho$) and other real space functions at the bond critical point (BCP) using Bader's quantum theory atoms in molecules (QTAIM)[13] as implemented by Multiwfn.[14] The natural bond orbital (NBO)[15] method was used to perform population analysis and gain further into bonding. The Extended Transition State - Natural Orbitals for Chemical Valence (ETS-NOCV)[16] analysis was also done using Multiwfn.

Table S3: Comparison of the selected observed (from SCXRD data) versus computed (from DFT optimized geometry) distances (d) in Å.

	d_{obs}	$d_{calc.}$
[(LX)Ca{N(SiMe$_3$)$_2$}]		
Ca-$C_{carbene}$	2.55	2.53
Ca---Flu(η^5)	2.46	2.45
Ca-N_{HMDS}	2.26	2.25
[(LX)CaI(thf)$_2$]		
Ca-$C_{carbene}$	2.62	2.60
Ca---Flu(η^5)	2.52	2.56
Ca-I	3.06	3.02
Ca-O1	2.45	2.42
Ca-O2	2.37	2.36
[(LX)Sr{N(SiMe$_3$)$_2$}(thf)]		
Sr-$C_{carbene}$	2.81	2.79
Sr---Flu(η^5)	2.67	2.66
Sr-N_{HMDS}	2.46	2.45
Sr-O	2.51	2.52
[(LX)SrI(thf)$_2$]		
Sr-$C_{carbene}$	2.75	2.74
Sr---Flu(η^5)	2.64	2.67
Sr-I	3.19	3.16
Sr-O1	2.57	2.56
Sr-O2	2.52	2.52

AIM analysis

Covalent and non-covalent interactions can be distinguished by the electron density(ρ) at the bond critical point (BCP). In the case of covalent interactions, the value of ρ is large (>0.1) while its

Laplacian $\nabla^2\rho$ at BCP is negative; non-covalent interactions have a small value of ρ with a positive value of $\nabla^2\rho$. Local electronic energy density, H_{BCP} can be used for further differentiation between covalent and non-covalent interactions along with the $\nabla^2\rho$ at BCP. Covalent interactions have $\nabla^2\rho < 0$ and $H_{BCP} < 0$, partially covalent interactions or strong electrostatic interactions have $\nabla^2\rho > 0$ and $H_{BCP} < 0$; whereas, weaker non-covalent interactions have $\nabla^2\rho > 0$ and $H_{BCP} > 0$.

Table S4: Selected topological parameters

interaction	ρ *10^{-1}	$\nabla^2\rho$ *10^{-1}	H_{BCP} *10^{-3} in a.u.
[(LX)Ca{N(SiMe$_3$)$_2$}]			
Ca-$C_{carbene}$	0.373	0.123	-0.247
Ca-C_{flu}	0.228	0.815	0.808
Ca-N_{HMDS}	0.575	2.371	-2.156
[(LX)CaI(thf)$_2$]			
Ca-$C_{carbene}$	0.322	0.103	0.270
Ca-C_{flu}	0.256	0.847	0.433
Ca-I	0.261	0.686	-0.588
[(LX)Sr{N(SiMe$_3$)$_2$}(thf)]			
Sr-$C_{carbene}$	0.273	0.801	0.373
Sr-C_{flu}	0.197	0.659	0.868
Sr-N_{HMDS}	0.461	1.619	-1.992
[(LX)SrI(thf)$_2$]			
Sr-$C_{carbene}$	0.300	0.868	-0.014
Sr-C_{flu}	0.229	0.719	0.471
Sr-I	0.247	0.623	-0.310

NBO analysis

The NBO method can describe an N-electron wavefunction in terms of localized orbitals which corresponds to the Lewis concept of chemical bonding. It provides a localized picture of bonding and donor-acceptor interactions. The second-order Fock matrix analysis provides the stabilization energy $E^{(2)}$ associated for the delocalization $i \rightarrow j$ for each donor (i) and acceptor (j) and is estimated as:

$$E(2) = \Delta E_{ij} = q_i \frac{F(i,j)^2}{\varepsilon_j - \varepsilon_i}$$

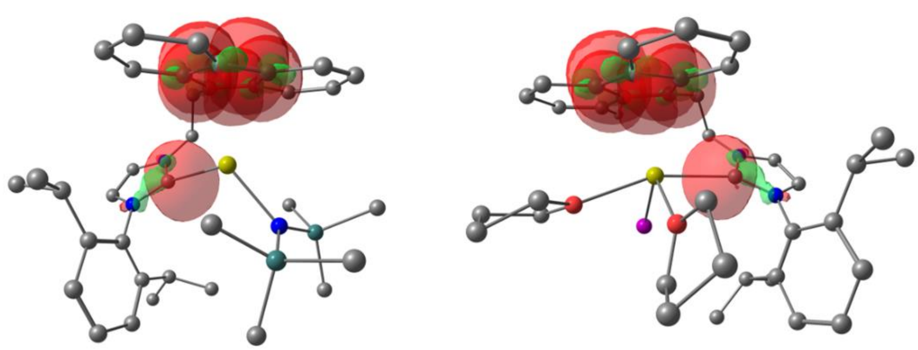
Table S5: Natural population and charges on selected atoms

Atom	Natural population	Natural charge
[(LX)Ca{N(SiMe$_3$)$_2$}]		
Ca	18.226	1.774
$C_{carbene}$	6.037	-0.037
C_{flu}	6.223	-0.223
N_{HMDS}	8.883	-1.883
[(LX)CaI(thf)$_2$]		
Ca	18.282	1.718
$C_{carbene}$	5.993	0.007
C_{flu}	6.247	-0.247
I	53.856	-0.856
[(LX)Sr{N(SiMe$_3$)$_2$}(thf)]		
Sr	36.188	1.812
$C_{carbene}$	6.011	-0.011
C_{flu}	6.218	-0.218
N_{HMDS}	8.881	-1.881
[(LX)SrI(thf)$_2$]		
Sr	36.254	1.746
$C_{carbene}$	5.989	0.011
C_{flu}	6.227	-0.227
I	53.870	-0.870

Table S6: Second-order perturbation theory analysis of Fock matrix in NBO basis

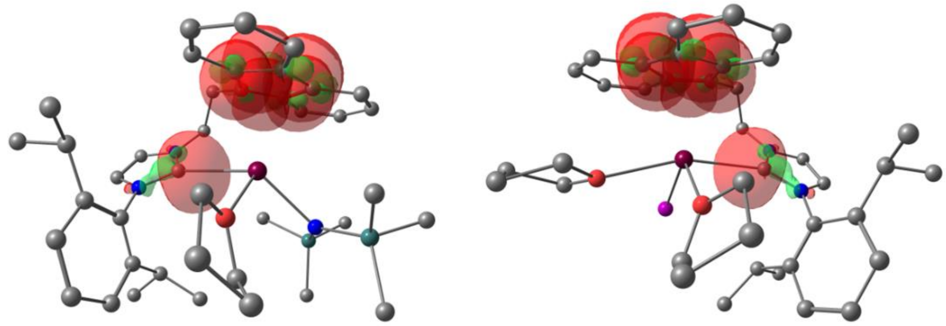
Donor NBO (i) / occupancy	Acceptor NBO (j) / occupancy	$E^{(2)}$ in kcal/mol
[(LX)Ca{N(SiMe$_3$)$_2$}]		
π (C7-C8) / 1.968	LP* Ca / 0.117	2.8
π (C7-C10) / 1.959	LP* Ca / 0.117	2.8
π (C8-C11) / 1.969	LP* Ca / 0.117	2.8
π (C9-C10) / 1.970	LP* Ca / 0.117	2.8
π (C9-C11) / 1.959	LP* Ca / 0.117	2.7
LP C17 / 1.880	LP* Ca / 0.117	15.9
LP N6 / 1.870	RY* Ca / 0.048	6.8
[(LX)CaI(thf)$_2$]		
π (C7-C11) / 1.968	LP* Ca / 0.157	2.9
π (C7-C14) / 1.959	LP* Ca / 0.157	2.5

π (C11-C21) / 1.968	LP* Ca / 0.157	2.9
π (C14-C38) / 1.969	LP* Ca / 0.157	2.4
π (C21-C38) / 1.958	LP* Ca / 0.157	2.5
LP C24 / 1.878	LP* Ca / 0.157	15.0
LP I / 1.986	LP* Ca / 0.157	29.4
LP I / 1.921	LP* Ca / 0.157	6.8
[(LX)Sr{N(SiMe$_3$)$_2$}(thf)]		
π (C8-C9) / 1.959	LP* Sr / 0.110	2.3
π (C8-C14) / 1.970	LP* Sr / 0.110	2.4
π (C9-C34) / 1.968	LP* Sr / 0.110	2.5
π (C14-C17) / 1.958	LP* Sr / 0.110	2.3
π (C17-C34) / 1.969	LP* Sr / 0.110	2.4
LP N6 / 1.873	RY* Sr / 0.027	7.0
LP C10 / 1.891	LP* Sr / 0.110	12.8
[(LX)SrI(thf)$_2$]		
π (C7-C8) / 1.968	LP* Sr / 0.147	2.3
π (C7-C13) / 1.959	LP* Sr / 0.147	2.1
π (C8-C10) / 1.969	LP* Sr / 0.147	2.2
π (C10-C12) / 1.959	LP* Sr / 0.147	2.0
π (C12-C13) / 1.970	LP* Sr / 0.147	2.0
LP C11 / 1.879	LP* Sr / 0.147	16.9
LP I / 1.927	LP* Sr / 0.147	27.9
LP I / 1.989	LP* Sr / 0.147	8.9



[(LX)Ca{NS(iMe$_3$)$_2$}] **[(LX)CaI(thf)$_2$]**

Figure S10. NBO plots showing pi orbitals of fluorenyl ring and lone pair of carbene donating to Ca^{2+} centre (iso value = 0.05).



[(LX)Sr{NS(iMe$_3$)$_2$}(thf)] **[(LX)SrI(thf)$_2$]**

Figure S11. NBO plots showing pi orbitals of fluorenyl ring and lone pair of carbene donating to Sr^{2+} centre (iso value = 0.05).

ETS-NOCV analysis

Total energy variation due to inter-fragment interaction between fragments *A* and *B* may be expressed as (fragments mentioned below are considered to be in complex geometry, so deformation energy due to distortion of fragment structure during combination is not taken into account in this context):

$\Delta E_{\text{int}} = E_{AB} - E_A - E_B = \Delta E_{\text{els}} + \Delta E_{\text{XC}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{orb}}$

where E_{AB} is the complex electronic energy, E_A and E_B are the electronic energies of fragments *A* and *B* at complex geometry respectively.

ΔE_{els} is the inter-fragment electrostatic interaction energy, ΔE_{XC} is the change in exchange-correlation (XC) energy, ΔE_{Pauli} is the Energy increase due to Pauli repulsion between electrons of the two fragments and ΔE_{orb} is the orbital interaction energy due to mix of fragment orbitals, which accounts for polarization effect and charge-transfer effect.

ΔE_{orb} is always a negative term and thus stabilizes the complex. The ETS-NOCV method focuses on gaining deep chemical insights into the ΔE_{orb} term.

Complexation energies ($\Delta E_{\text{complex}}$) are calculated using the supermolecular model. For the model complex $[(LX)M]^+$ it is calculated as

$\Delta E_{\text{complex}} = E_{\text{LM}} - (E_{\text{L}} + E_{\text{M}})$

where E is the electronic energy of the respective fragments. Complexation energy along with basis set superposition error (BSSE) were determined using the counterpoise (CP) method at B3LYP-D3/B2/B3LYP-D3/B1 level of theory. ΔE_{int} is calculated as:

$\Delta E_{\text{int}} = \Delta E_{\text{complex}} + \text{BSSE}$

ΔE_{orb} was calculated for $[(LX)M]^+$ at B3LYP-D3/B2 level using multiwfn.

Table S7: Energy decomposition analysis of $[(LX)M]^+$ (energy values in kcal/mol)

complex	$\Delta E_{complex}$	BSSE	ΔE_{int}	ΔE_{orb}
$[LCa]^+$	-378.18	0.93	-377.25	-103.00
$[LSr]^+$	-345.21	0.48	-344.73	-97.39

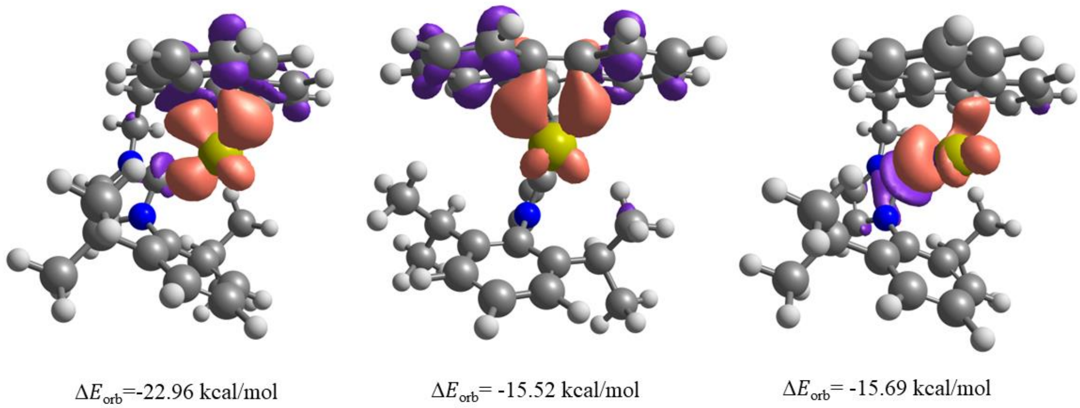


Figure S12. Important NOCV pairs and their contributions to ΔE_{orb} for $[(LX)Ca]^+$ (the colours orange and violet represent electron-deficient and electron-rich orbitals respectively, iso value=0.005).

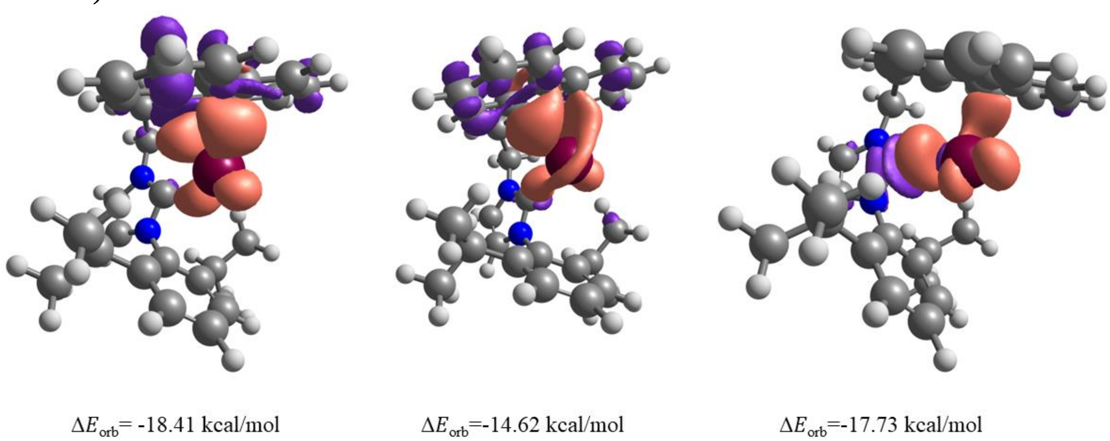


Figure S13. Important NOCV pairs and their contributions to ΔE_{orb} for $[(LX)Sr]^+$.

Cartesian Coordinates of optimized structures and their electronic energies at B3LYP-D3/B2 level of theory

$[(LX)Ca\{N(SiMe_3)_2\}]$

E= -2823.29697133 a.u.

20	0.887878000	-0.305240000	-0.081981000
14	2.318527000	2.825844000	0.490240000

14	0.808031000	2.118801000	-2.114533000
7	-2.391592000	-0.533153000	1.307441000
7	-0.952743000	-1.292698000	2.695220000
7	1.360491000	1.844421000	-0.529881000
6	2.776584000	-1.952689000	0.972248000
6	1.545184000	-2.587763000	1.309415000
6	1.832660000	-2.703262000	-1.012164000
6	2.957146000	-1.990964000	-0.463792000
6	0.987712000	-3.085724000	0.098365000
6	-2.983008000	0.269438000	0.265145000
6	-3.114841000	-1.102908000	2.348132000
1	-4.189373000	-1.085545000	2.377991000
6	-2.201438000	-1.591222000	3.221738000
1	-2.327362000	-2.103631000	4.159721000
6	-1.046535000	-0.637603000	1.508887000
6	1.032343000	-2.831479000	2.694439000
1	1.862628000	-3.098083000	3.359903000
1	0.349637000	-3.686907000	2.700578000
6	-0.182219000	-3.838115000	-0.164757000
1	-0.830835000	-4.143704000	0.649363000
6	0.317739000	-1.633373000	3.343617000
1	0.094328000	-1.839055000	4.392789000
1	0.954204000	-0.747587000	3.310382000
6	4.097911000	-1.413353000	-1.050791000
1	4.233565000	-1.446961000	-2.126587000
6	1.488785000	-3.073774000	-2.325654000
1	2.127901000	-2.791458000	-3.155866000
6	3.766943000	-1.321998000	1.765650000
1	3.663225000	-1.283744000	2.844890000
6	0.347750000	-3.820987000	-2.545724000
1	0.080637000	-4.121580000	-3.551635000
6	-3.391222000	-0.336930000	-0.934791000
6	-3.127841000	1.643357000	0.508327000
6	4.878639000	-0.776466000	1.157511000
1	5.637616000	-0.297031000	1.765258000
6	-0.474415000	-4.207461000	-1.460945000
1	-1.354785000	-4.809497000	-1.656185000
6	-2.653674000	2.299703000	1.793833000
1	-2.255291000	1.523449000	2.447701000
6	5.048867000	-0.817505000	-0.245906000

1	5.930982000	-0.371360000	-0.688355000
6	4.143500000	2.843763000	-0.000854000
1	4.537796000	1.826724000	-0.051859000
1	4.752112000	3.413151000	0.709805000
1	4.270704000	3.297911000	-0.988578000
6	2.202177000	2.111615000	2.247598000
1	1.161155000	2.053904000	2.581496000
1	2.751365000	2.721520000	2.971520000
1	2.637386000	1.106919000	2.284692000
6	-3.812013000	2.977785000	2.541383000
1	-4.244092000	3.792347000	1.954207000
1	-3.456126000	3.400729000	3.484570000
1	-4.610652000	2.265862000	2.765561000
6	-3.971963000	0.485606000	-1.902628000
1	-4.292021000	0.057927000	-2.842854000
6	-0.104038000	0.515815000	-2.650172000
1	-0.515931000	0.648752000	-3.654254000
1	-0.970993000	0.296638000	-2.013107000
6	-3.228824000	-1.830219000	-1.170813000
1	-2.350454000	-2.163246000	-0.613003000
6	-3.710641000	2.421497000	-0.494672000
1	-3.824735000	3.487518000	-0.341538000
6	1.777272000	4.641576000	0.549606000
1	1.907162000	5.110749000	-0.431125000
1	2.385167000	5.206951000	1.263787000
1	0.729180000	4.755986000	0.833191000
6	-4.130796000	1.849041000	-1.686279000
1	-4.574161000	2.468984000	-2.456756000
6	-0.460238000	3.507776000	-2.289556000
1	-1.336531000	3.307359000	-1.669082000
1	-0.796621000	3.618477000	-3.325724000
1	-0.036228000	4.463641000	-1.969625000
6	-1.509409000	3.281238000	1.503225000
1	-0.704042000	2.791274000	0.954066000
1	-1.102402000	3.679861000	2.436329000
1	-1.855608000	4.126356000	0.901826000
6	-4.445669000	-2.603131000	-0.630406000
1	-4.596305000	-2.428398000	0.435880000
1	-4.307836000	-3.677659000	-0.778445000
1	-5.356394000	-2.300514000	-1.155183000

6	2.179544000	2.412743000	-3.381553000
1	2.922011000	1.610445000	-3.335938000
1	2.702127000	3.351336000	-3.172045000
1	1.794955000	2.468189000	-4.405151000
6	-2.993656000	-2.182514000	-2.644512000
1	-3.874869000	-1.972831000	-3.256561000
1	-2.779024000	-3.247325000	-2.736852000
1	-2.144782000	-1.636072000	-3.058213000
1	0.529258000	-0.380071000	-2.719607000

[(LX)CaI(thf)$_2$]

E= -2712.74245725 a.u.

53	-1.340636000	-3.021364000	-0.296997000
20	-0.971147000	-0.031881000	-0.089005000
8	0.325010000	0.654324000	1.758550000
8	-2.533507000	-0.069563000	1.753903000
7	1.053485000	-0.744729000	-2.782978000
7	2.550692000	-0.488013000	-1.281978000
6	-2.819311000	0.884474000	-1.945023000
6	-0.929821000	0.487407000	-3.683469000
1	-0.222632000	1.171153000	-4.164674000
1	-1.733770000	0.318407000	-4.410115000
6	-1.505156000	1.122755000	-2.453510000
6	2.270005000	-0.989686000	-3.400925000
1	2.347574000	-1.262043000	-4.439026000
6	-3.108483000	1.832751000	-0.895981000
6	-0.233425000	-0.864749000	-3.474552000
1	-0.859127000	-1.547483000	-2.895171000
1	-0.027224000	-1.340037000	-4.435943000
6	3.238477000	-0.356772000	-0.024509000
6	2.551222000	-2.764950000	0.489149000
1	1.672785000	-2.526786000	-0.111652000
6	-0.984814000	2.240786000	-1.741052000
6	3.252296000	-1.462707000	0.845998000
6	3.943807000	0.827975000	0.247093000
6	1.194344000	-0.433360000	-1.465947000
6	-3.798497000	-0.079999000	-2.283180000
1	-3.593189000	-0.828504000	-3.039790000
6	0.570506000	-0.134761000	2.948471000

1	1.390746000	-0.821996000	2.739432000
1	-0.337287000	-0.700858000	3.157929000
6	4.685461000	0.883929000	1.430808000
1	5.247020000	1.778875000	1.666581000
6	3.220684000	-0.834524000	-2.453284000
1	4.286845000	-0.960240000	-2.489619000
6	0.240400000	2.943728000	-1.841968000
1	0.984885000	2.636541000	-2.568397000
6	-4.370193000	1.839814000	-0.280449000
1	-4.608919000	2.588515000	0.468104000
6	-1.951943000	2.674409000	-0.754310000
6	1.695427000	1.947536000	3.203321000
1	1.708882000	2.923400000	3.690601000
1	2.724206000	1.636135000	3.021409000
6	3.962578000	1.997808000	-0.727950000
1	3.070738000	1.919088000	-1.353111000
6	4.712829000	-0.191233000	2.309536000
1	5.295120000	-0.128207000	3.222033000
6	3.998079000	-1.347564000	2.022200000
1	4.030335000	-2.180143000	2.712729000
6	-5.021920000	-0.059015000	-1.644381000
1	-5.774398000	-0.793293000	-1.909452000
6	0.466115000	4.042332000	-1.036538000
1	1.392797000	4.595464000	-1.137167000
6	-1.685577000	3.790656000	0.055934000
1	-2.426270000	4.131589000	0.772788000
6	3.927188000	3.368132000	-0.035305000
1	3.081920000	3.464117000	0.646028000
1	3.839743000	4.156134000	-0.786726000
1	4.843996000	3.559559000	0.528136000
6	0.956254000	0.877294000	4.020439000
1	1.577899000	0.430995000	4.797849000
1	0.065997000	1.298481000	4.495774000
6	2.047794000	-3.556088000	1.700967000
1	2.868760000	-3.953844000	2.305338000
1	1.447824000	-4.397271000	1.351085000
1	1.402331000	-2.952273000	2.340404000
6	-0.490553000	4.473046000	-0.087718000
1	-0.284702000	5.345974000	0.521023000
6	-5.318253000	0.905491000	-0.653892000

1	-6.299183000	0.912044000	-0.192553000
6	5.201789000	1.926180000	-1.640243000
1	6.117269000	1.994511000	-1.045617000
1	5.197205000	2.754706000	-2.353712000
1	5.238544000	0.996440000	-2.207169000
6	0.912563000	1.975350000	1.893920000
1	0.101211000	2.704499000	1.901949000
1	1.526191000	2.154689000	1.014518000
6	-2.749250000	1.028689000	2.664103000
1	-3.127140000	1.884830000	2.100172000
1	-1.788533000	1.292202000	3.102379000
6	3.480516000	-3.650609000	-0.362522000
1	3.801280000	-3.142964000	-1.273001000
1	2.956651000	-4.563960000	-0.654849000
1	4.372934000	-3.931943000	0.205251000
6	-4.656726000	-0.374859000	2.784888000
1	-5.212607000	-1.122920000	3.351690000
1	-5.368406000	0.233532000	2.223447000
6	-3.775722000	0.519399000	3.667473000
1	-3.285643000	-0.071501000	4.446874000
1	-4.325941000	1.330876000	4.146593000
6	-3.648641000	-1.013051000	1.832916000
1	-3.246810000	-1.956664000	2.203383000
1	-4.034826000	-1.164928000	0.827213000

[(LX)Sr{N(SiMe$_3$)$_2$}(thf)]

E= -2409.00003680 a.u.

38	-0.713052000	-0.352661000	0.063904000
14	-3.297078000	1.753526000	1.355230000
14	-2.758991000	1.957990000	-1.629601000
7	2.768860000	-0.229019000	-1.605176000
7	1.474770000	-1.506902000	-2.719145000
7	-2.385941000	1.432702000	-0.052205000
8	0.636104000	0.917878000	1.779736000
6	-2.484479000	-2.642522000	0.492689000
6	-2.075189000	-2.799917000	-0.883553000
6	1.483174000	-0.698209000	-1.624496000
6	-3.820321000	-2.334265000	0.800444000
1	-4.135486000	-2.234866000	1.833307000

6	4.062218000	0.185128000	0.431325000
6	-1.324253000	-2.888678000	1.308250000
6	-1.121322000	-2.871149000	2.698779000
1	-1.945390000	-2.640788000	3.365443000
6	-0.228830000	-3.204842000	0.410056000
6	3.290322000	0.689538000	-0.630352000
6	3.522824000	-0.715905000	-2.666521000
1	4.545130000	-0.426861000	-2.828118000
6	3.049138000	2.059025000	-0.806550000
6	1.041788000	-3.485453000	0.970199000
1	1.880708000	-3.728952000	0.326446000
6	0.130470000	-3.163624000	3.212105000
1	0.290971000	-3.170643000	4.283886000
6	3.589586000	2.939170000	0.135268000
1	3.426253000	4.004283000	0.022633000
6	2.701966000	-1.532971000	-3.365252000
1	2.876026000	-2.113745000	-4.254351000
6	4.410453000	-1.293360000	0.533008000
1	3.658614000	-1.850351000	-0.029539000
6	-3.036553000	-2.619219000	-1.907172000
1	-2.762061000	-2.742222000	-2.949703000
6	-0.686455000	-3.119403000	-0.933463000
6	-4.339581000	-2.311789000	-1.569488000
1	-5.077435000	-2.179010000	-2.352786000
6	5.786692000	-1.554524000	-0.109350000
1	6.570619000	-1.027042000	0.441468000
1	5.823907000	-1.217525000	-1.145737000
1	6.018662000	-2.622718000	-0.092484000
6	0.337478000	-2.327000000	-3.144080000
1	0.579633000	-2.700927000	-4.141187000
1	-0.534377000	-1.680785000	-3.239778000
6	4.336029000	2.467629000	1.206526000
1	4.746361000	3.164853000	1.928171000
6	4.571398000	1.104676000	1.350465000
1	5.168063000	0.753068000	2.182515000
6	2.280364000	2.596698000	-2.002335000
1	1.881874000	1.746512000	-2.556081000
6	-4.736377000	-2.169581000	-0.221411000
1	-5.767185000	-1.929492000	0.008419000
6	0.046944000	-3.494503000	-2.183031000

1	-0.544074000	-4.226191000	-2.749940000
1	0.994014000	-3.987389000	-1.943896000
6	1.202186000	-3.474245000	2.342478000
1	2.169005000	-3.717933000	2.767320000
6	0.503303000	2.359949000	1.895841000
1	-0.424729000	2.633803000	1.396873000
1	1.347758000	2.825274000	1.385316000
6	-5.158552000	1.440073000	1.206022000
1	-5.641887000	2.184400000	0.567008000
1	-5.641918000	1.485150000	2.187934000
1	-5.350149000	0.455693000	0.773531000
6	-3.135261000	3.542707000	1.979958000
1	-2.104293000	3.813852000	2.224547000
1	-3.742297000	3.705551000	2.877128000
1	-3.480499000	4.245099000	1.215143000
6	1.293958000	0.385548000	2.959859000
1	2.207706000	-0.111030000	2.640839000
1	0.625361000	-0.352893000	3.407311000
6	-2.696530000	0.628699000	2.768944000
1	-2.927259000	-0.418646000	2.560309000
1	-3.199694000	0.888448000	3.705554000
1	-1.621781000	0.704576000	2.949036000
6	4.403265000	-1.835105000	1.967476000
1	4.612347000	-2.907568000	1.953685000
1	3.434968000	-1.697337000	2.446101000
1	5.171040000	-1.363378000	2.586041000
6	0.541928000	2.629854000	3.391393000
1	-0.440059000	2.455916000	3.835881000
1	0.844644000	3.653394000	3.617376000
6	3.224182000	3.360349000	-2.946662000
1	3.646978000	4.241348000	-2.455844000
1	2.682146000	3.696680000	-3.834282000
1	4.053682000	2.727476000	-3.271650000
6	-1.564071000	1.094841000	-2.843592000
1	-1.671556000	1.507940000	-3.851126000
1	-1.818540000	0.030753000	-2.914527000
6	1.559766000	1.584581000	3.874567000
1	1.441644000	1.328081000	4.927987000
1	2.576990000	1.953256000	3.722802000
6	1.086851000	3.465969000	-1.586788000

1	0.384894000	2.914001000	-0.960786000
1	0.541841000	3.802343000	-2.470871000
1	1.404868000	4.354507000	-1.034414000
6	-2.602979000	3.833498000	-1.874257000
1	-3.409872000	4.346167000	-1.340613000
1	-2.677851000	4.116307000	-2.929827000
1	-1.659280000	4.219577000	-1.482674000
1	-0.505673000	1.181999000	-2.577300000
6	-4.482083000	1.492860000	-2.261207000
1	-5.268026000	2.040128000	-1.734708000
1	-4.582003000	1.714366000	-3.329535000
1	-4.665732000	0.425727000	-2.114168000

[(LX)SrI(thf)$_2$]

E= -2065.85923391 a.u.

53	-1.578299000	-3.103920000	-0.042356000
38	-0.933823000	-0.012201000	-0.026779000
8	0.427285000	0.935735000	1.875527000
8	-2.621080000	0.272032000	1.884429000
7	1.204907000	-1.140520000	-2.687688000
7	2.677687000	-0.824950000	-1.174465000
6	-2.600615000	0.804806000	-2.231116000
6	-1.260151000	0.941240000	-2.702264000
6	3.318683000	-0.548551000	0.082066000
6	-0.719400000	2.101581000	-2.080174000
6	1.335085000	-0.708108000	-1.405981000
6	-1.705522000	2.669634000	-1.182846000
6	-2.887687000	1.858357000	-1.283947000
6	0.541651000	2.738272000	-2.186678000
1	1.303544000	2.330692000	-2.842516000
6	-3.602143000	-0.159143000	-2.501520000
1	-3.403601000	-0.982349000	-3.178217000
6	3.356589000	-1.322527000	-2.284466000
1	4.415178000	-1.506564000	-2.278232000
6	-4.160827000	1.953696000	-0.697677000
1	-4.391905000	2.773612000	-0.025060000
6	2.420741000	-1.515707000	-3.241302000
1	2.507784000	-1.895351000	-4.244453000

6	3.120163000	-1.442527000	1.152466000
6	-4.862296000	0.234085000	2.682886000
1	-5.527678000	-0.386461000	3.284448000
1	-5.463751000	0.777482000	1.951490000
6	-0.072175000	-1.237132000	-3.402802000
1	-0.767838000	-1.791383000	-2.768263000
1	0.114911000	-1.844916000	-4.290660000
6	-1.419213000	3.840888000	-0.462327000
1	-2.171041000	4.276782000	0.188529000
6	-0.649338000	0.131211000	-3.806176000
1	0.138602000	0.704704000	-4.305242000
1	-1.411706000	-0.066291000	-4.569792000
6	-4.835965000	-0.048381000	-1.892496000
1	-5.601186000	-0.787322000	-2.101750000
6	-0.187964000	4.455162000	-0.613275000
1	0.032831000	5.372442000	-0.079509000
6	4.811560000	0.792499000	1.397290000
1	5.468220000	1.647114000	1.502836000
6	-5.125361000	1.010422000	-1.000516000
1	-6.113666000	1.082299000	-0.561031000
6	0.784524000	3.897557000	-1.476905000
1	1.739158000	4.399039000	-1.586837000
6	1.249193000	2.125502000	1.701419000
1	0.600027000	2.918425000	1.329528000
1	2.005943000	1.904006000	0.952384000
6	4.379749000	1.524901000	-0.986555000
1	3.601106000	1.333007000	-1.726791000
6	4.151792000	0.577139000	0.182907000
6	2.263035000	-2.689374000	0.996699000
1	1.409993000	-2.442125000	0.362832000
6	3.791332000	-1.172062000	2.346923000
1	3.665920000	-1.841038000	3.187963000
6	5.745487000	1.254443000	-1.643364000
1	6.557660000	1.457179000	-0.939504000
1	5.884640000	1.897760000	-2.516336000
1	5.841213000	0.217209000	-1.968454000
6	1.847708000	2.431542000	3.077207000
1	2.857987000	2.025682000	3.145599000
1	1.894061000	3.503854000	3.270856000
6	4.633682000	-0.071924000	2.467872000

1	5.154577000	0.109080000	3.401533000
6	-3.795987000	-0.593713000	1.969663000
1	-3.503518000	-1.485792000	2.525699000
1	-4.077753000	-0.886568000	0.959406000
6	-2.862843000	1.508533000	2.587409000
1	-3.113240000	2.286087000	1.860411000
1	-1.941797000	1.788402000	3.097964000
6	4.274979000	3.003835000	-0.585888000
1	3.309977000	3.229541000	-0.132605000
1	4.381091000	3.634718000	-1.472119000
1	5.062376000	3.291174000	0.115553000
6	3.054287000	-3.799081000	0.279409000
1	3.410208000	-3.474545000	-0.699269000
1	2.412916000	-4.670825000	0.130455000
1	3.919833000	-4.102997000	0.876415000
6	-4.031196000	1.215802000	3.520696000
1	-3.675203000	0.735213000	4.436567000
1	-4.578636000	2.118370000	3.796963000
6	1.689573000	-3.224545000	2.311913000
1	2.464188000	-3.652207000	2.956053000
1	0.962884000	-4.006421000	2.087436000
1	1.163526000	-2.449217000	2.872758000
6	0.911622000	1.689016000	4.043995000
1	1.391419000	1.432781000	4.989747000
1	0.023486000	2.288914000	4.261430000
6	0.538130000	0.456229000	3.232069000
1	1.326965000	-0.298794000	3.277622000
1	-0.417652000	0.001699000	3.494333000

[(LX)Ca]$^+$

E= -1949.47444253 a.u.

20	-0.775174000	-0.175652000	-0.688726000
7	1.883820000	-0.557846000	1.189748000
7	0.310448000	-0.569902000	2.641901000
6	-3.050179000	-0.416830000	0.566139000
6	-2.317087000	0.581298000	1.279553000
6	-2.777344000	1.386462000	-0.879236000
6	-3.317937000	0.054637000	-0.778318000
6	-2.181606000	1.701785000	0.402639000

6	2.449747000	-0.442752000	-0.131087000
6	2.507993000	-0.627501000	2.426399000
1	3.576769000	-0.660802000	2.542789000
6	1.505355000	-0.639903000	3.345668000
1	1.543060000	-0.694877000	4.420044000
6	0.529766000	-0.523155000	1.312018000
6	-1.935855000	0.567091000	2.734856000
1	-2.842102000	0.523553000	3.351572000
1	-1.446331000	1.510571000	2.989216000
6	-1.493849000	2.935282000	0.544970000
1	-1.048599000	3.209305000	1.494384000
6	-1.037820000	-0.580762000	3.230156000
1	-0.914653000	-0.505104000	4.310817000
1	-1.486817000	-1.551250000	3.016704000
6	-3.924283000	-0.795136000	-1.727916000
1	-4.139098000	-0.432203000	-2.727233000
6	-2.671955000	2.289298000	-1.960061000
1	-3.137612000	2.058799000	-2.912133000
6	-3.437176000	-1.740025000	0.906537000
1	-3.299845000	-2.113362000	1.914013000
6	-1.990822000	3.477387000	-1.783907000
1	-1.915494000	4.185467000	-2.599528000
6	2.911316000	0.814727000	-0.562025000
6	2.356538000	-1.557633000	-0.987973000
6	-4.027136000	-2.544819000	-0.046458000
1	-4.331384000	-3.550089000	0.220192000
6	-1.408900000	3.794210000	-0.531000000
1	-0.894605000	4.741145000	-0.416694000
6	1.885927000	-2.924670000	-0.502106000
1	1.888738000	-2.910895000	0.589011000
6	-4.265157000	-2.083230000	-1.363654000
1	-4.742270000	-2.740565000	-2.079630000
6	2.838990000	-4.044378000	-0.950824000
1	2.808917000	-4.198719000	-2.031831000
1	2.555902000	-4.986399000	-0.476553000
1	3.869290000	-3.817529000	-0.670901000
6	3.294884000	0.932718000	-1.901616000
1	3.665501000	1.881791000	-2.266605000
6	3.009980000	2.003752000	0.379782000
1	2.421324000	1.776509000	1.270931000

6	2.724539000	-1.373065000	-2.325642000
1	2.667850000	-2.206037000	-3.015048000
6	3.191062000	-0.142643000	-2.776435000
1	3.483710000	-0.024619000	-3.812828000
6	0.444379000	-3.228130000	-0.955417000
1	-0.289089000	-2.638660000	-0.388819000
1	0.181875000	-4.268957000	-0.755356000
1	0.314491000	-3.061054000	-2.029204000
6	4.469863000	2.208193000	0.822970000
1	4.875845000	1.310124000	1.294345000
1	4.538511000	3.030199000	1.538945000
1	5.105768000	2.450260000	-0.032392000
6	2.430427000	3.287968000	-0.230731000
1	3.014658000	3.633544000	-1.086522000
1	2.440531000	4.087806000	0.513033000
1	1.396810000	3.148291000	-0.555440000

$[(LX)Sr]^+$

E= -1302.59697831 a.u.

38	-0.688014000	-0.274784000	-0.848202000
7	2.030680000	-0.302938000	1.213506000
7	0.468966000	-0.709638000	2.618552000
6	-3.386601000	-0.287825000	-0.696776000
6	-2.977887000	-0.866023000	0.568569000
6	0.702348000	-0.590892000	1.294508000
6	-3.933354000	-1.100043000	-1.711925000
1	-4.255824000	-0.660112000	-2.649741000
6	2.674341000	1.273424000	-0.549465000
6	-3.023057000	1.105507000	-0.665727000
6	-3.116515000	2.133711000	-1.627887000
1	-3.607309000	1.951281000	-2.578008000
6	-2.394802000	1.352703000	0.614754000
6	2.609366000	-0.055218000	-0.083478000
6	2.621545000	-0.244668000	2.467702000
1	3.666529000	-0.037237000	2.614353000
6	2.941666000	-1.162406000	-0.884907000
6	-1.889498000	2.651091000	0.882556000
1	-1.432598000	2.875746000	1.839630000
6	-2.604783000	3.383195000	-1.334301000

1	-2.686253000	4.186064000	-2.056233000
6	3.339660000	-0.908436000	-2.202202000
1	3.605290000	-1.735339000	-2.848489000
6	1.626954000	-0.506324000	3.356833000
1	1.648552000	-0.570477000	4.431141000
6	2.348741000	2.452720000	0.354548000
1	1.681988000	2.095002000	1.143703000
6	-3.168863000	-2.258902000	0.766758000
1	-2.922328000	-2.720993000	1.715193000
6	-2.337657000	0.135755000	1.362121000
6	-3.701152000	-3.027051000	-0.250311000
1	-3.853043000	-4.088315000	-0.092306000
6	3.635163000	2.969991000	1.025845000
1	4.334923000	3.346828000	0.275552000
1	4.141473000	2.183427000	1.588384000
1	3.403107000	3.785227000	1.714719000
6	-0.857791000	-1.017204000	3.170093000
1	-0.749208000	-1.066871000	4.253866000
1	-1.140198000	-2.010683000	2.821569000
6	3.411450000	0.391528000	-2.689643000
1	3.729352000	0.567546000	-3.710372000
6	3.088987000	1.469509000	-1.870870000
1	3.160009000	2.475089000	-2.263817000
6	2.846058000	-2.590913000	-0.368017000
1	2.773282000	-2.548908000	0.720126000
6	-4.076783000	-2.457808000	-1.491242000
1	-4.506107000	-3.089623000	-2.258616000
6	-1.931498000	0.023629000	2.805837000
1	-2.810254000	-0.228230000	3.412706000
1	-1.591013000	0.998390000	3.164541000
6	-2.000698000	3.635003000	-0.077778000
1	-1.625840000	4.629621000	0.132811000
6	1.626262000	3.592324000	-0.375551000
1	1.318939000	4.353323000	0.344166000
1	0.724912000	3.247701000	-0.887792000
1	2.271817000	4.081615000	-1.108180000
6	4.092948000	-3.418319000	-0.715254000
1	4.179487000	-3.597637000	-1.789427000
1	4.041212000	-4.392484000	-0.224558000
1	5.003738000	-2.917219000	-0.381846000

6	1.570363000	-3.278210000	-0.888778000
1	0.672749000	-2.797800000	-0.480905000
1	1.531978000	-4.321844000	-0.569278000
1	1.528172000	-3.262368000	-1.981697000

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