SUPPORTING INFORMATION

Contents

1 Supporting experimental data

1.1 ^{1}H, $^{19}F\{^{1}H\}$, and $^{13}C\{^{1}H\}$ NMR spectra of synthesized compounds

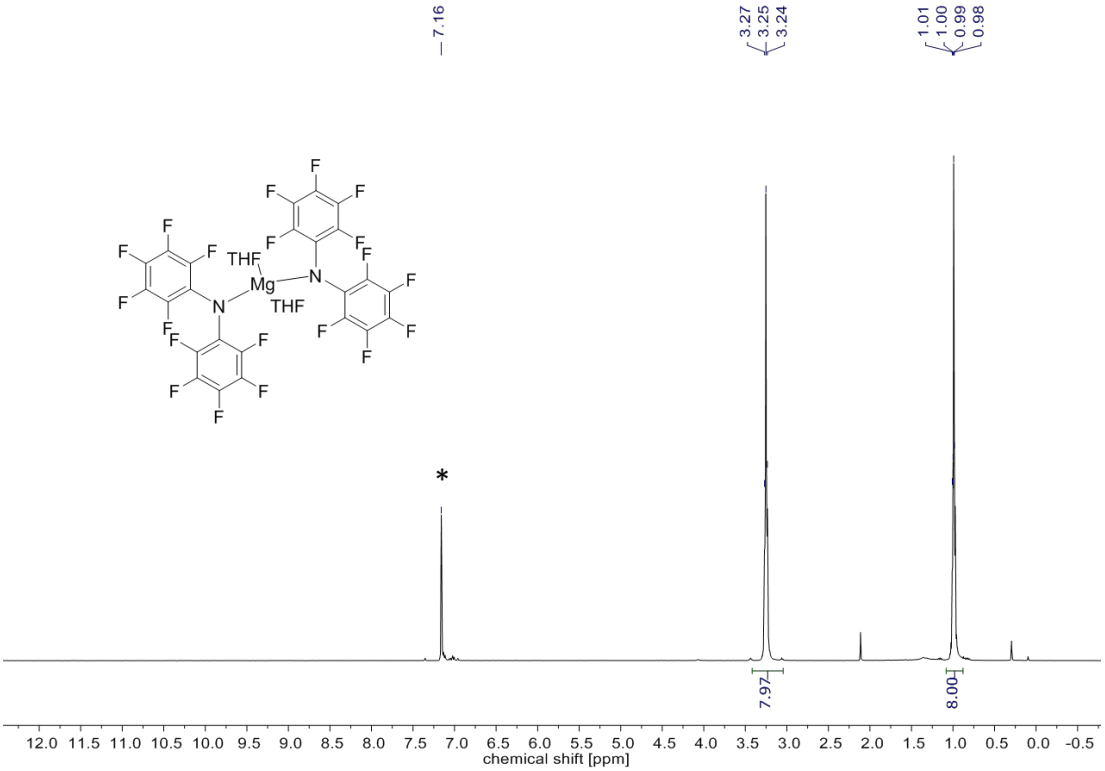

Figure S 1 ^{1}H NMR (400 MHz, C_6D_6, rt) of $MgN^{F}_{2}\cdot(THF)_2$.

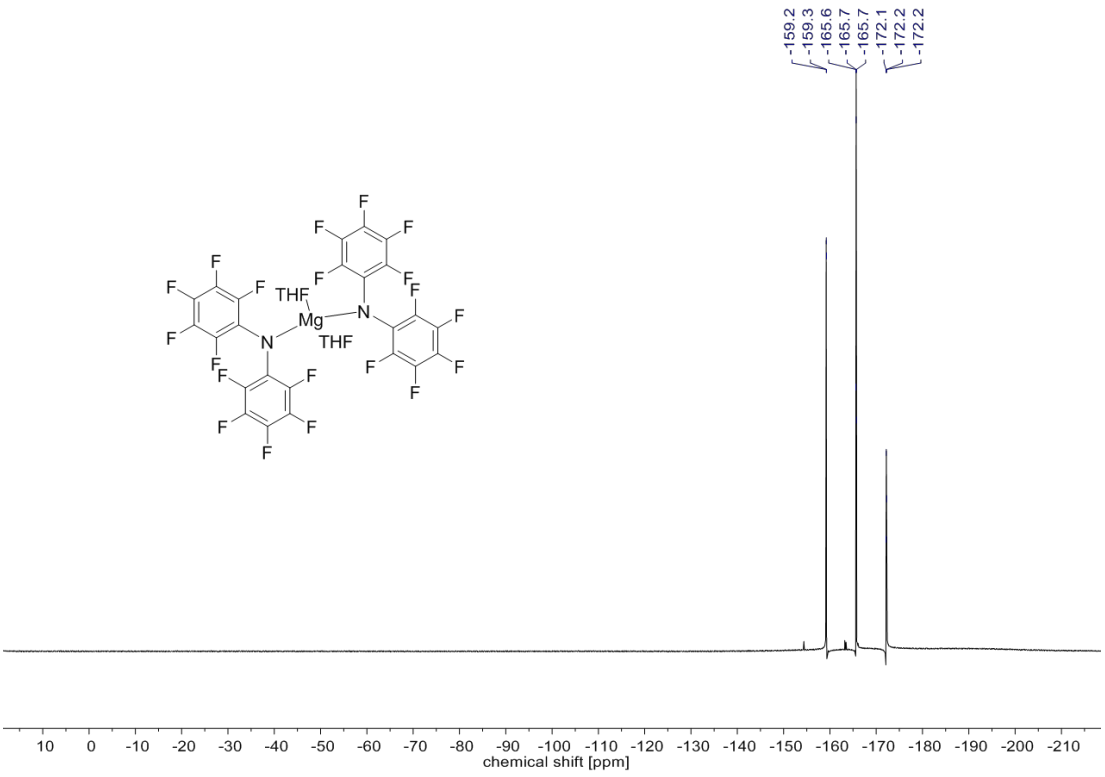

Figure S 2 $^{19}F\{^{1}H\}$ NMR (376 MHz, C_6D_6, rt) of $MgN^{F}_{2}\cdot(THF)_2$.

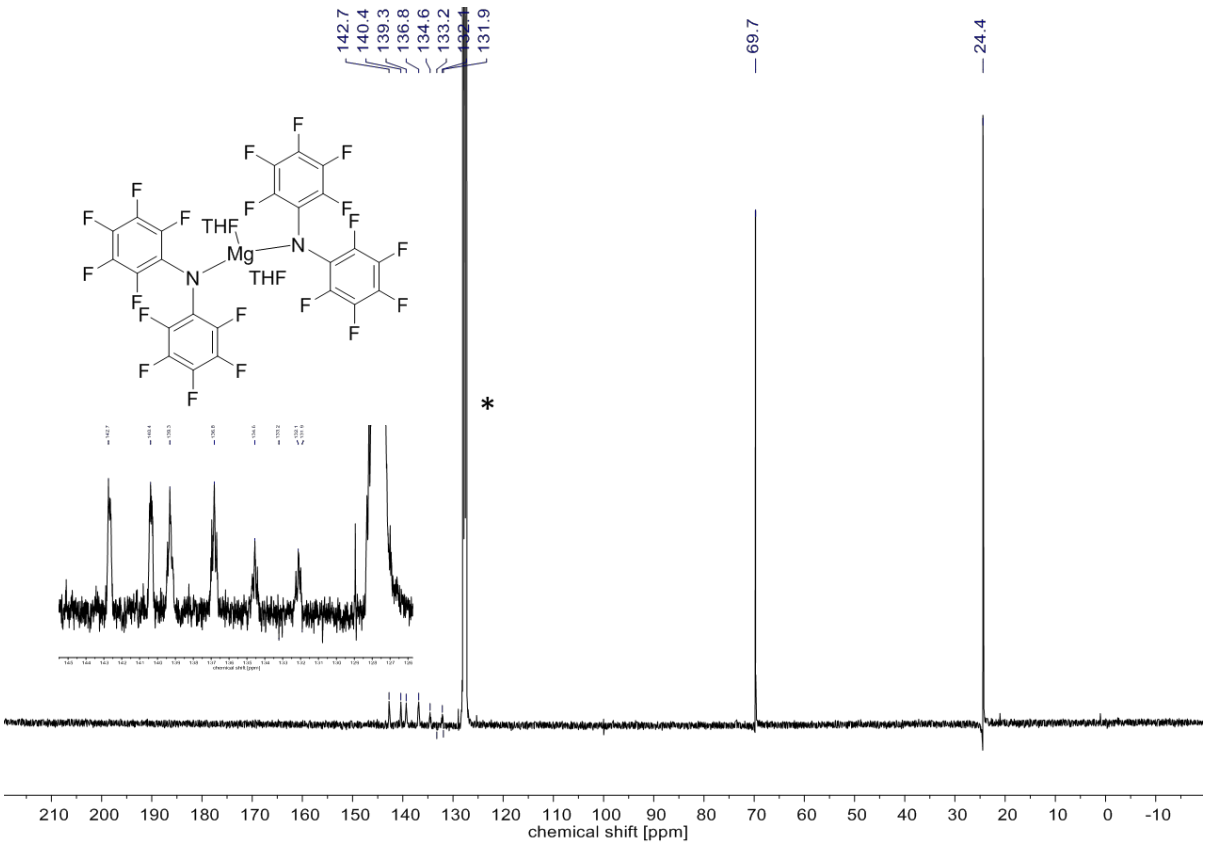

Figure S 3 $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, rt) of $MgN^{F}_{2}(THF)$.

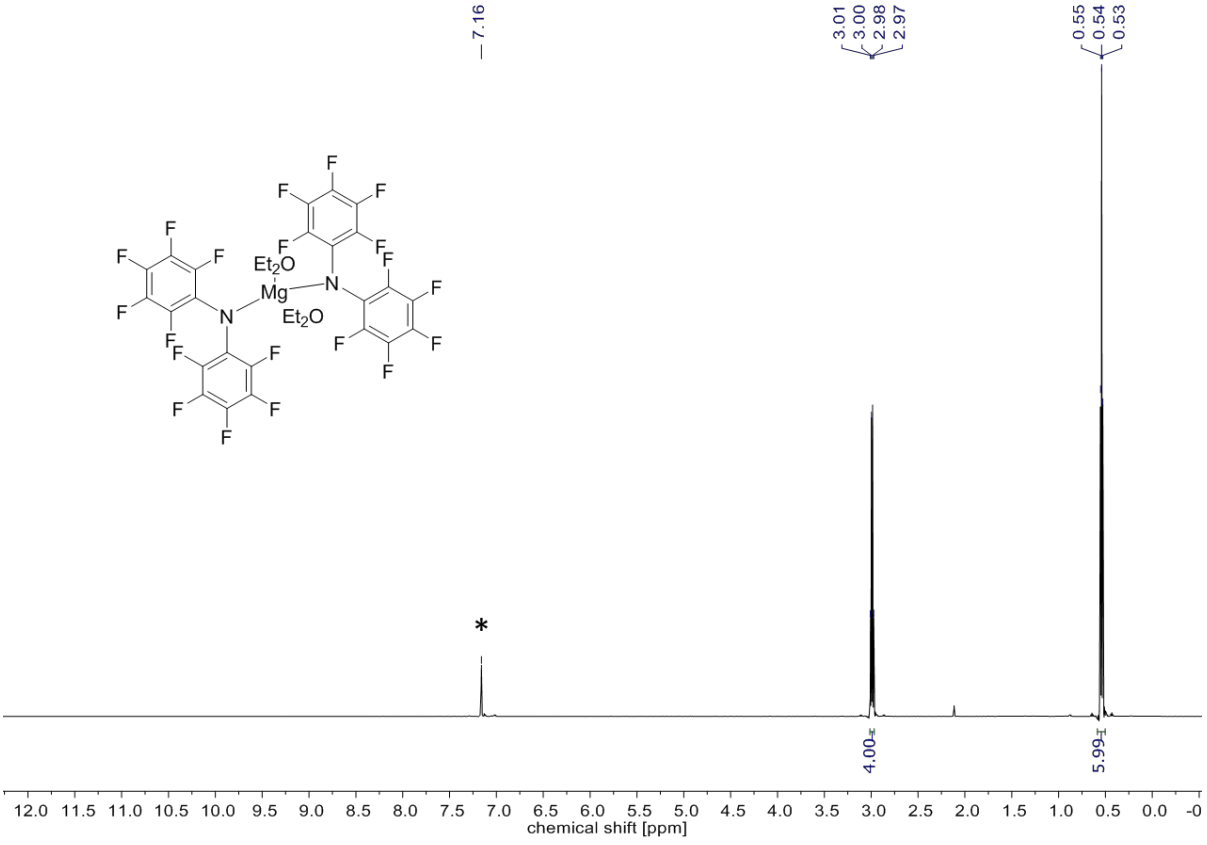

Figure S 4 ^{1}H NMR (600 MHz, C_6D_6, rt) of $MgN^{F}_{2}\cdot(Et_2O)_2$.

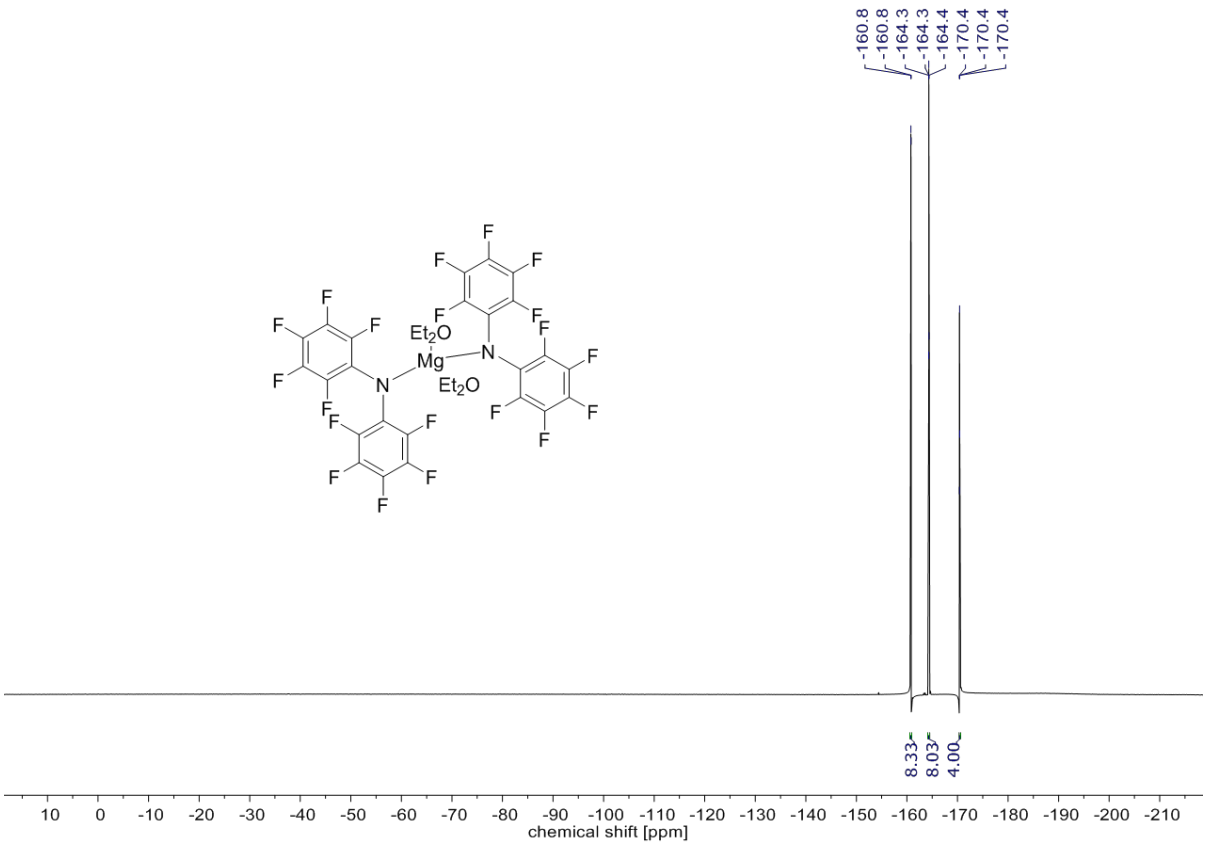

Figure S5 $^{19}F\{^{1}H\}$ NMR (565 MHz, C_6D_6, rt) of $MgN^{F}_{2}\cdot(Et_2O)$.

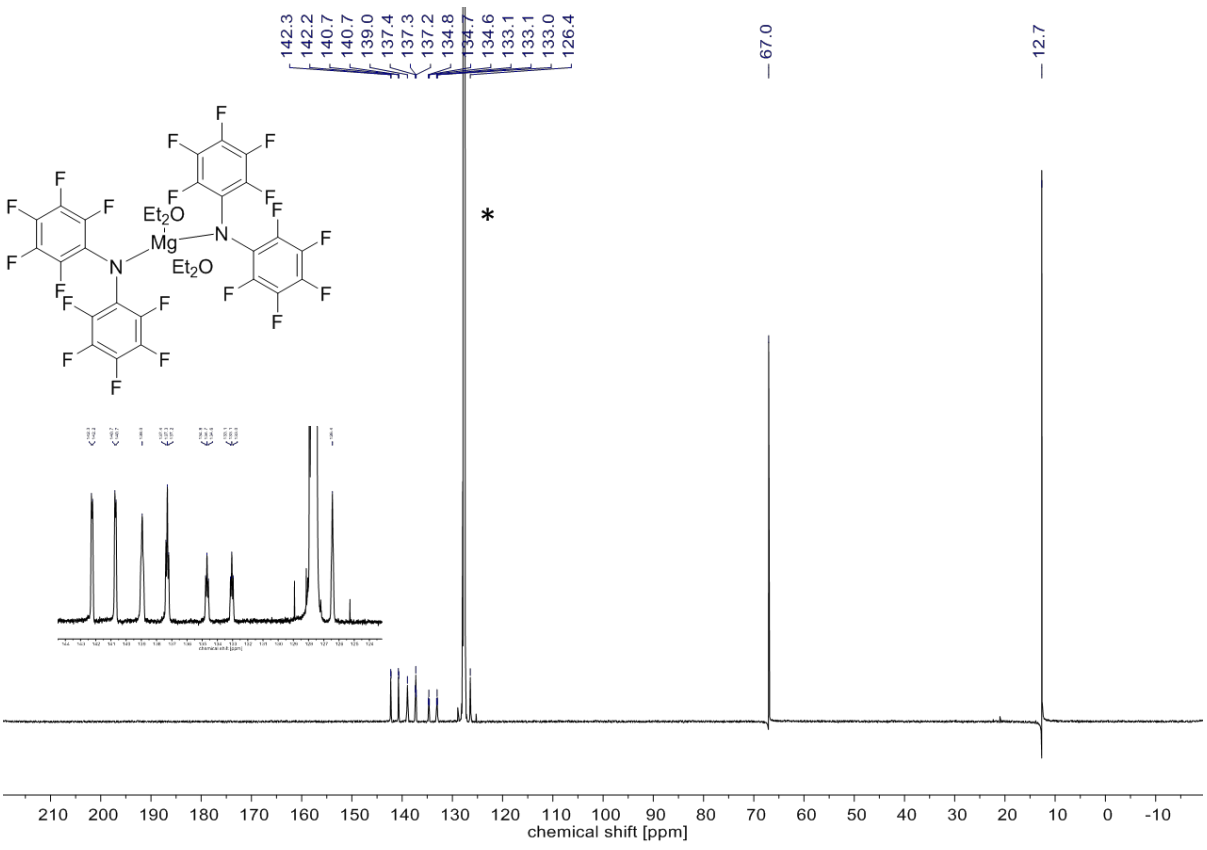

Figure S6 $^{13}C\{^{1}H\}$ NMR (151 MHz, C_6D_6, rt) of $MgN^{F}_{2}\cdot(Et_2O)_2$.

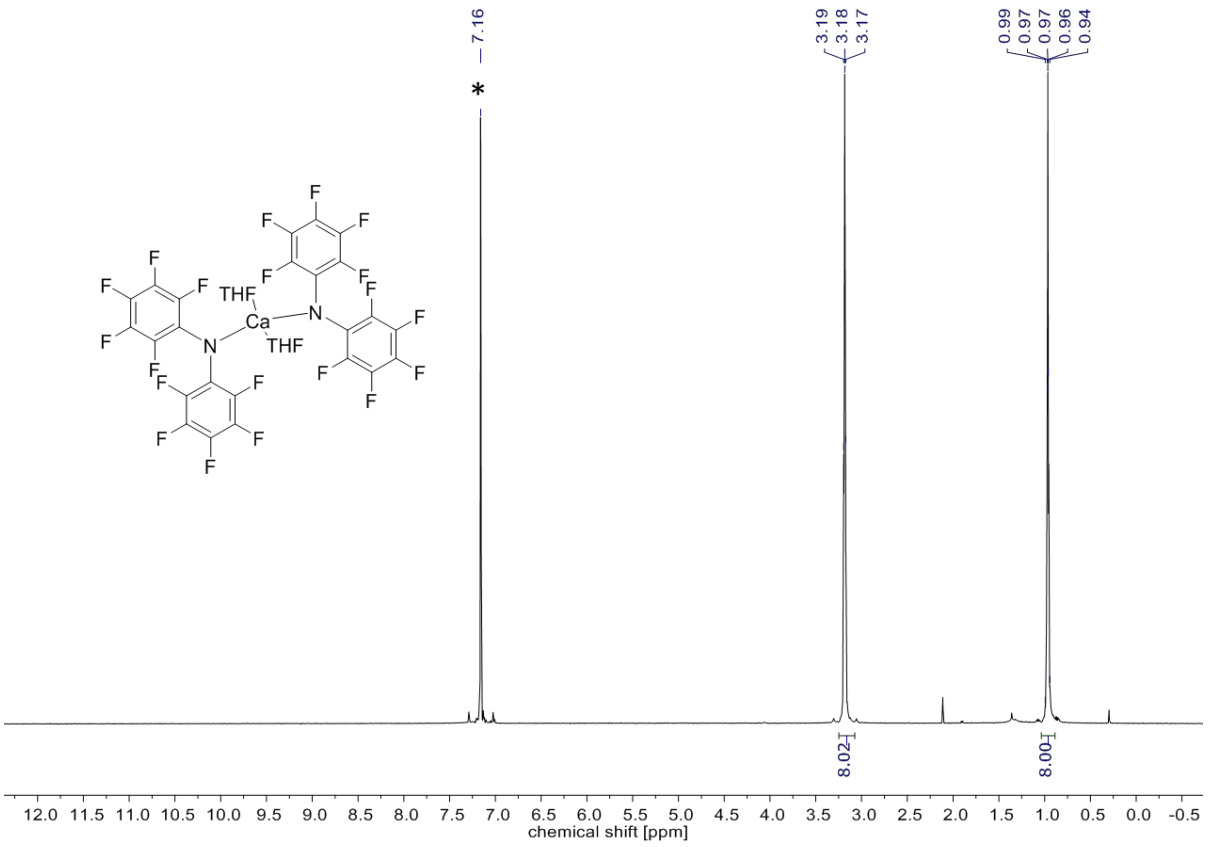

Figure S 7 ^{1}H NMR (400 MHz, C_6D_6, rt) of $CaN^{F}_{2}(THF)$.

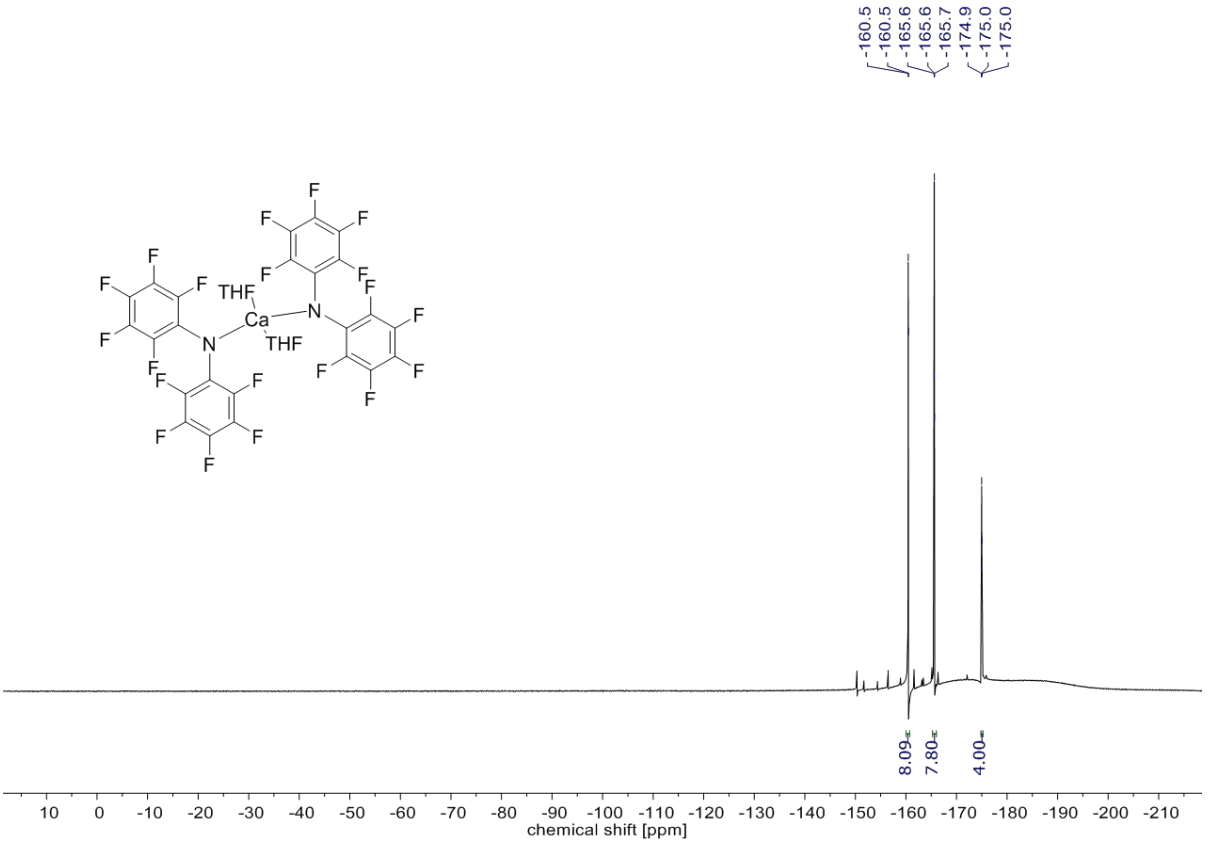

Figure S 8 ^{19}F {^{1}H} NMR (376 MHz, C_6D_6, rt) of $CaN^{F}_{2}\cdot(THF)_2$.

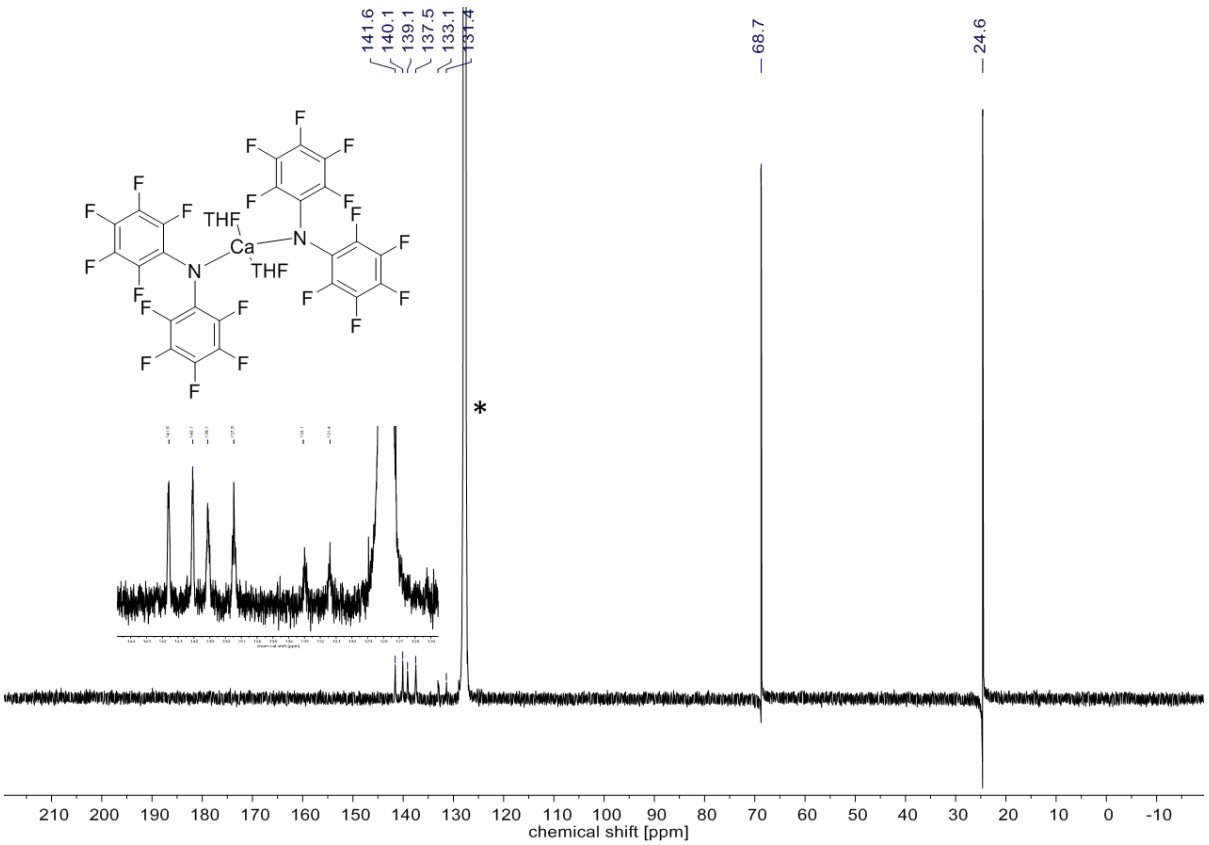

Figure S 9 $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, rt) of $CaN^{F}_{2}\cdot(THF)_2$.

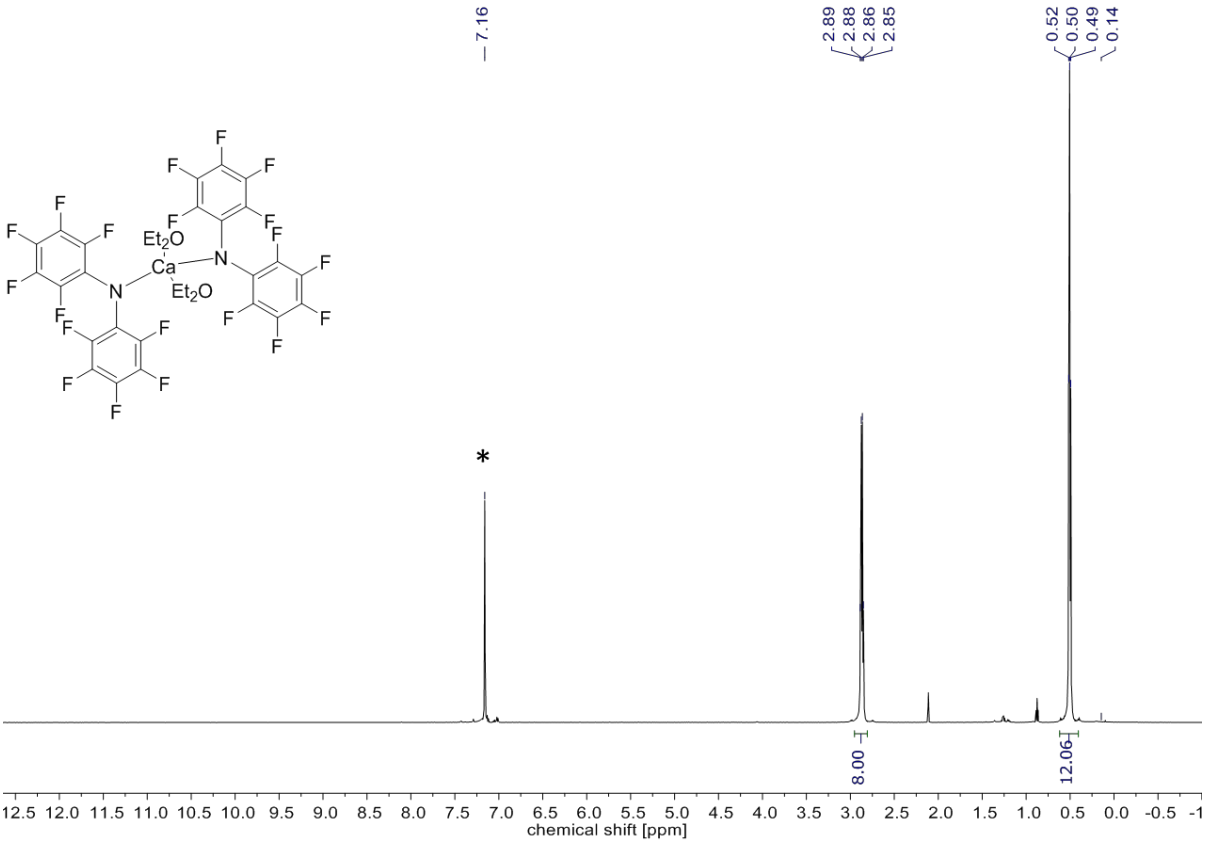

Figure S 10 ^{1}H NMR (600 MHz, C_6D_6, rt) of $CaN^{F}_{2}\cdot(Et_2O)_2$.

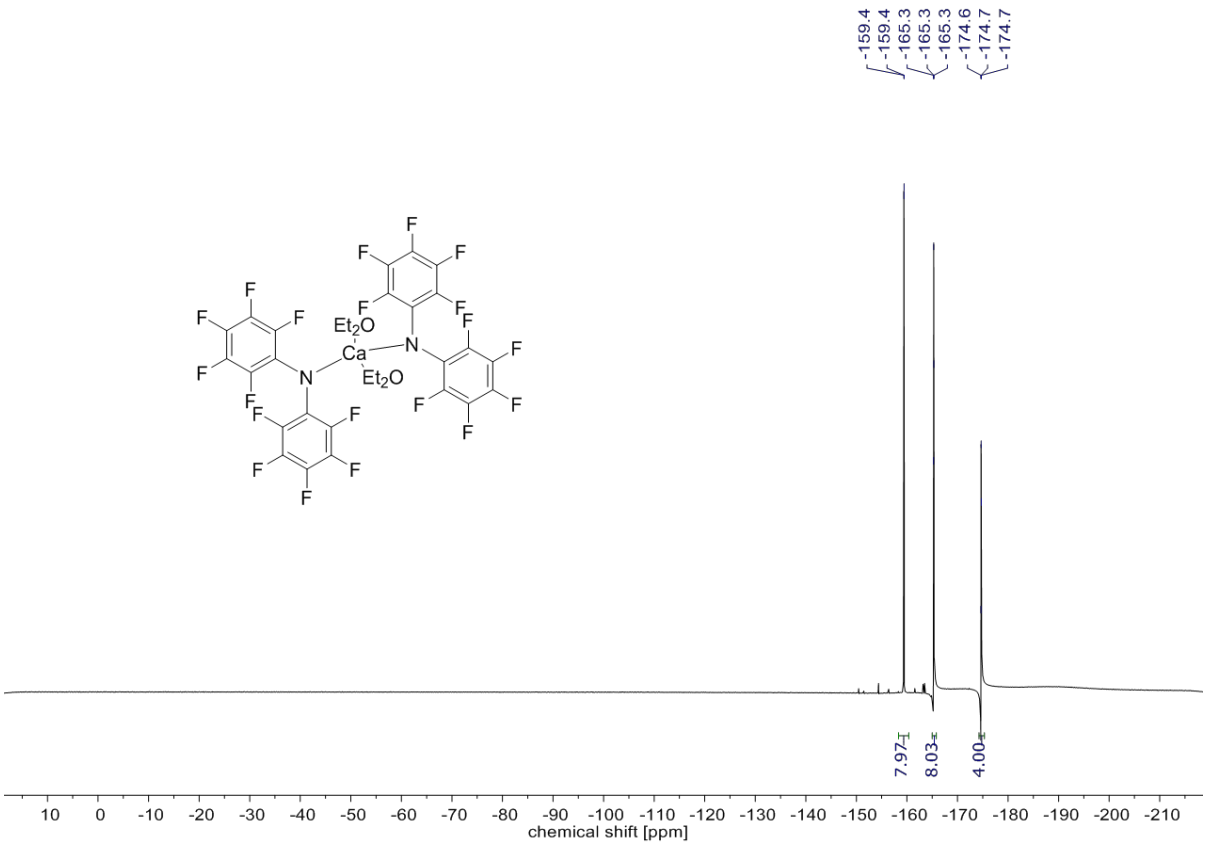

Figure S11 $^{19}F\{^{1}H\}$ NMR (565 MHz, C_6D_6, rt) of $CaN^{F}_{2}\cdot(Et_2O)$.

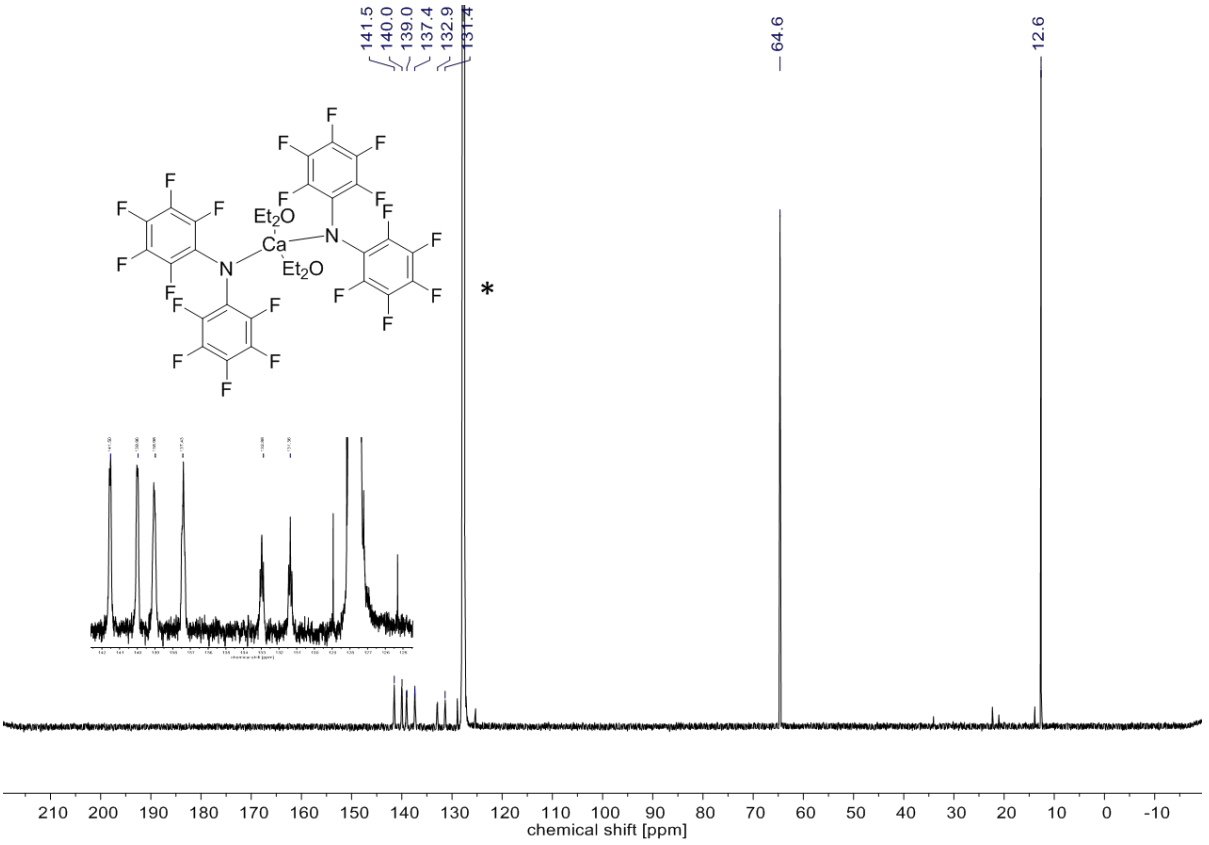

Figure S12 $^{13}C\{^{1}H\}$ NMR (151 MHz, C_6D_6, rt) of $CaN^{F}_{2}\cdot(Et_2O)_2$.

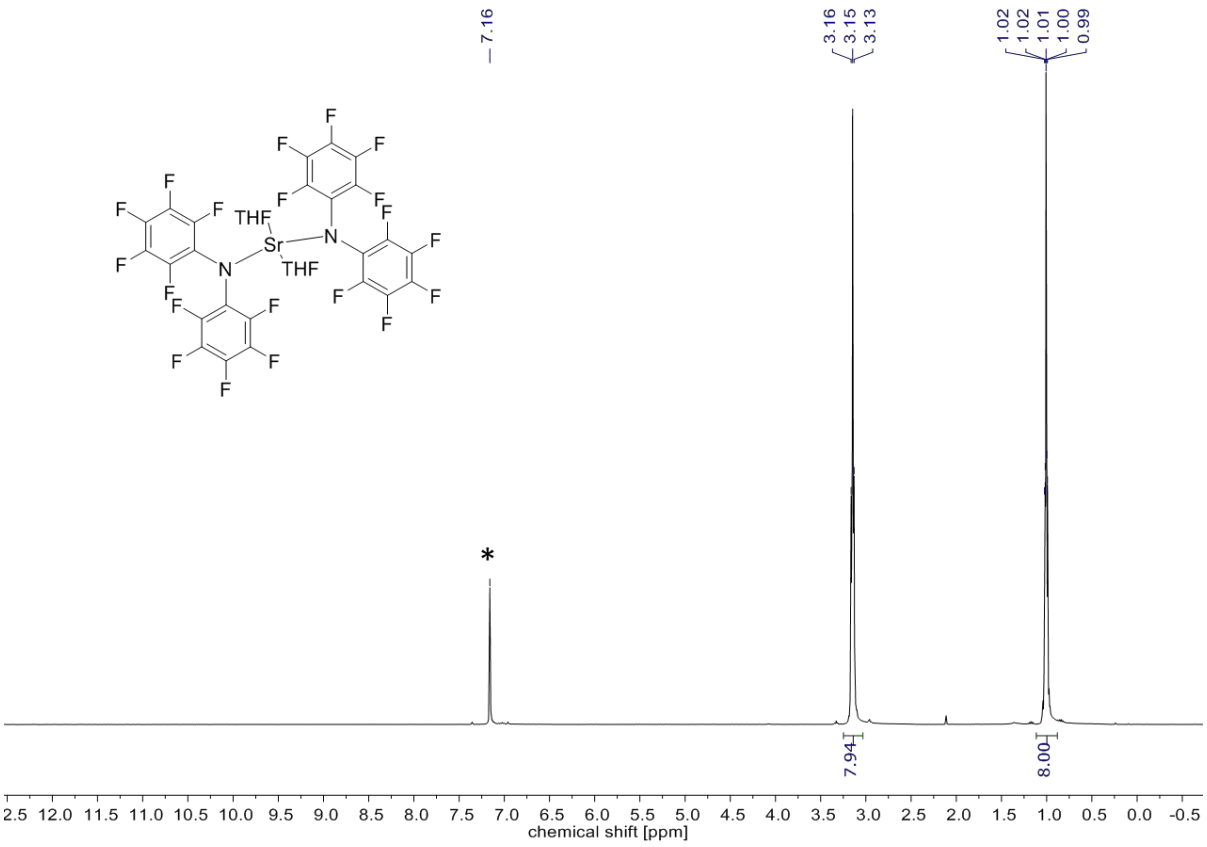

Figure S 13 ^{1}H NMR (400 MHz, C_6D_6, rt) of $SrN^{F}_{2}(THF)_2$.

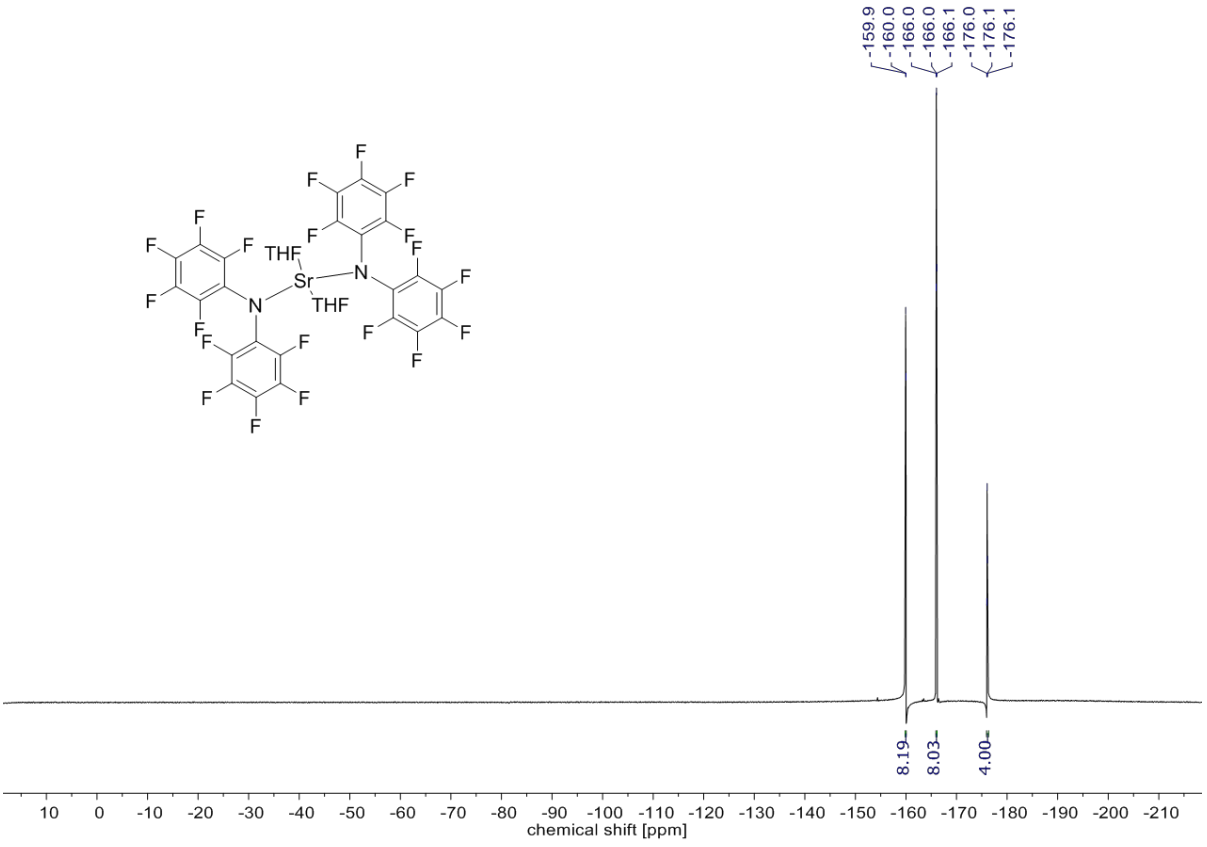

Figure S 14 ^{19}F {^{1}H} NMR (376 MHz, C_6D_6, rt) of $SrN^{F}_{2}\cdot(THF)_2$.

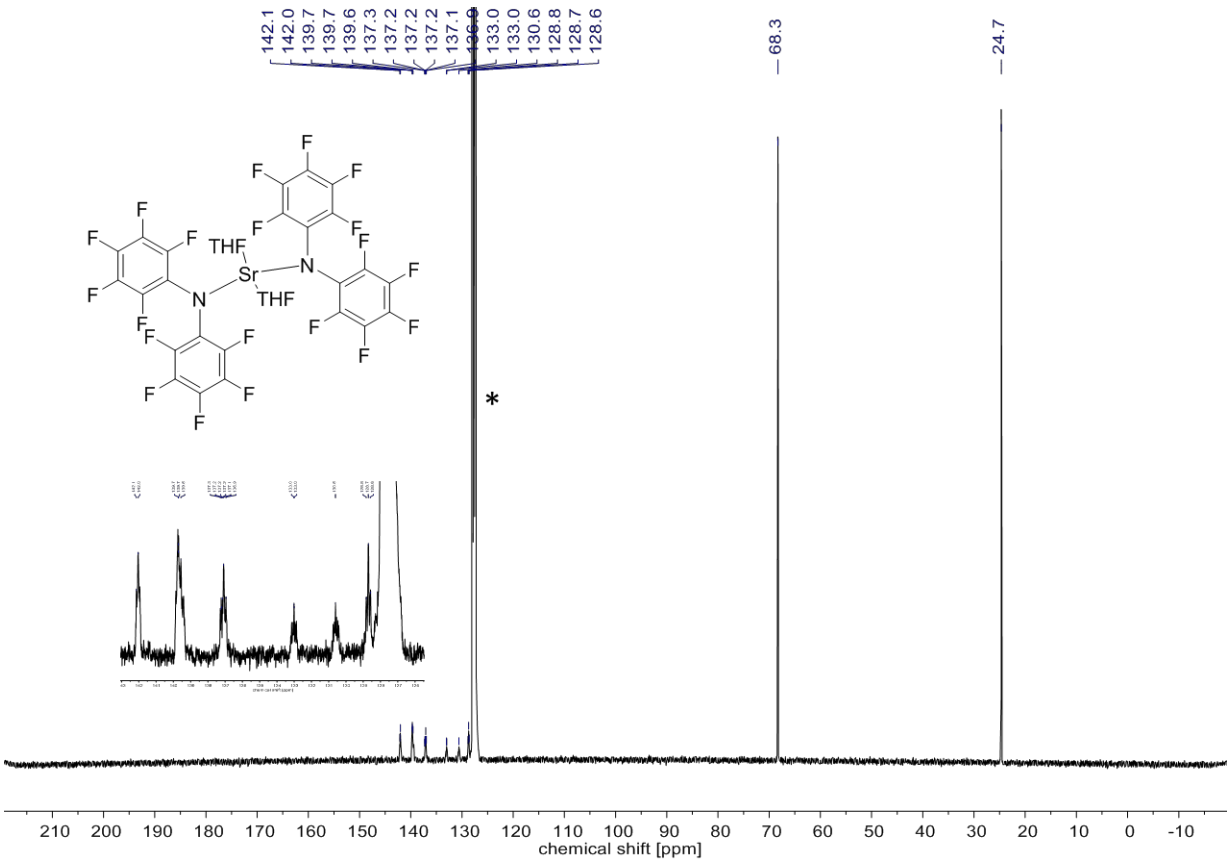

Figure S 15 ^{13}C {^{1}H} NMR (101 MHz, C_6D_6, rt) of $SrN^F_2 \cdot (THF)_2$.

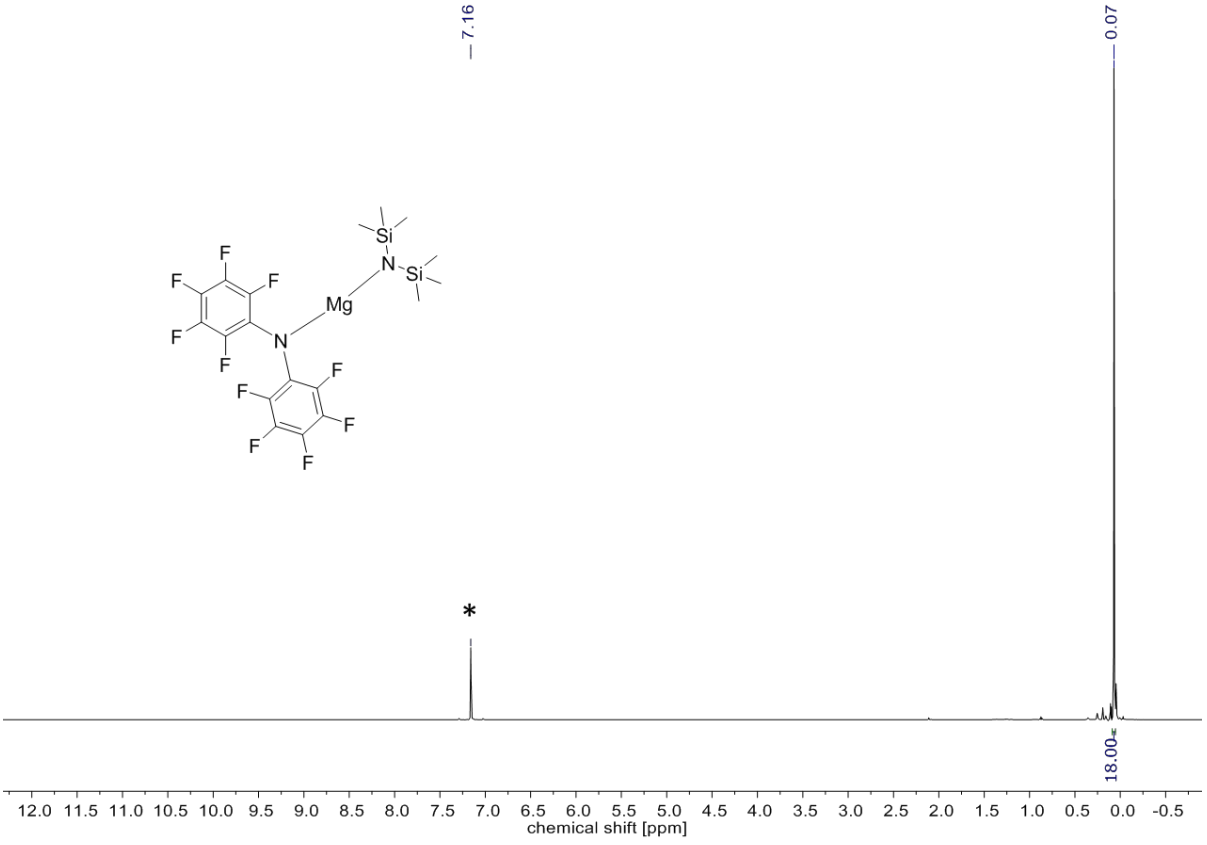

Figure S 16 ^{1}H NMR (600 MHz, C_6D_6, rt) of $(N^FMgN'')_2$.

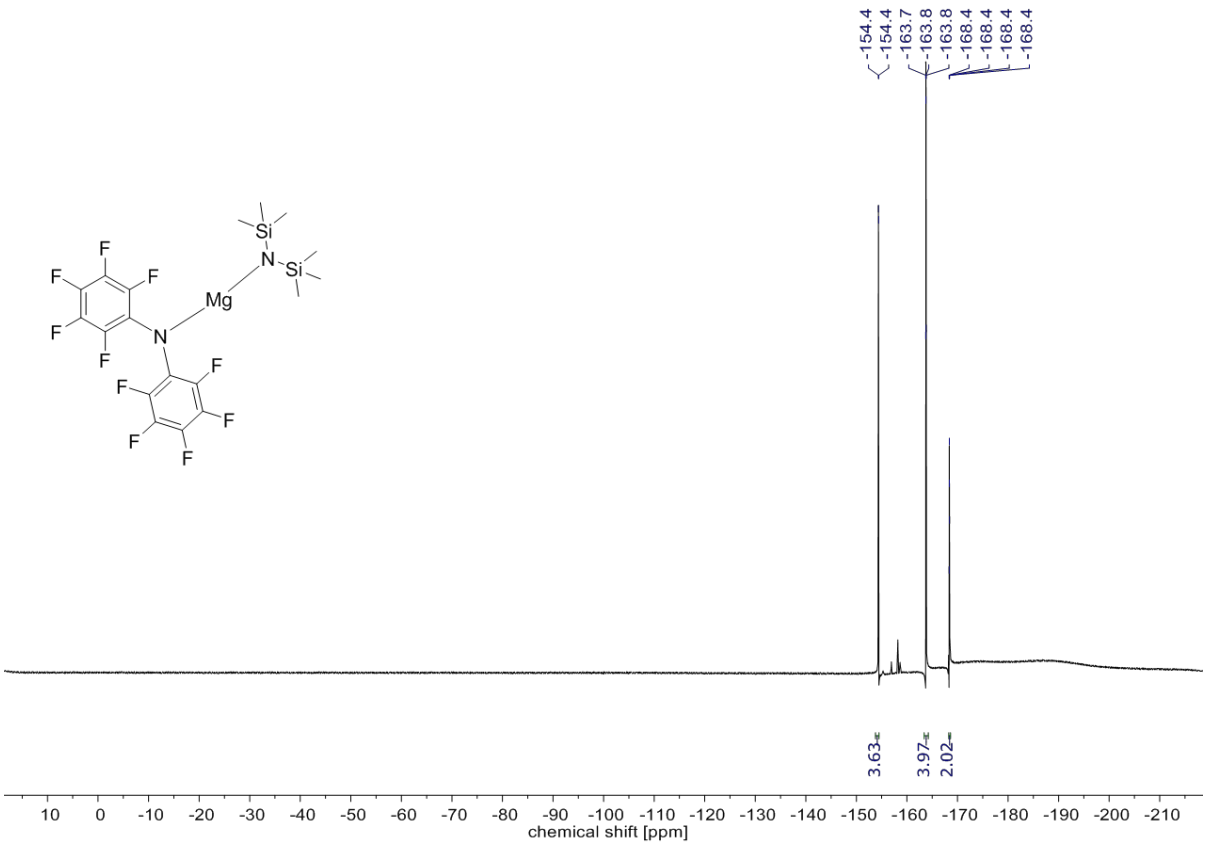

Figure S17 $^{19}F\{^{1}H\}$ NMR (565 MHz, C_6D_6, rt) of $(N^{F}MgN'')_2$.

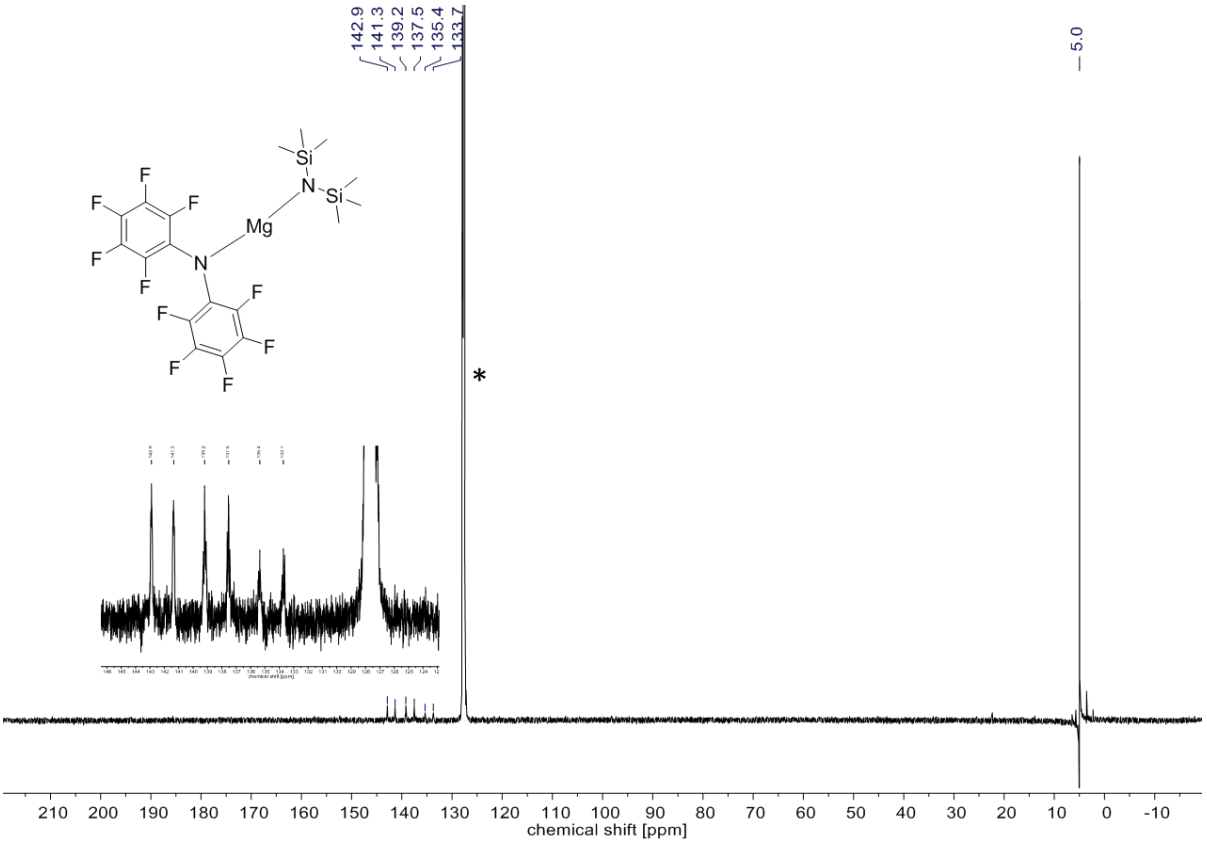

Figure S18 $^{13}C\{^{1}H\}$ NMR (151 MHz, C_6D_6, rt) of $(N^{F}MgN'')_2$.

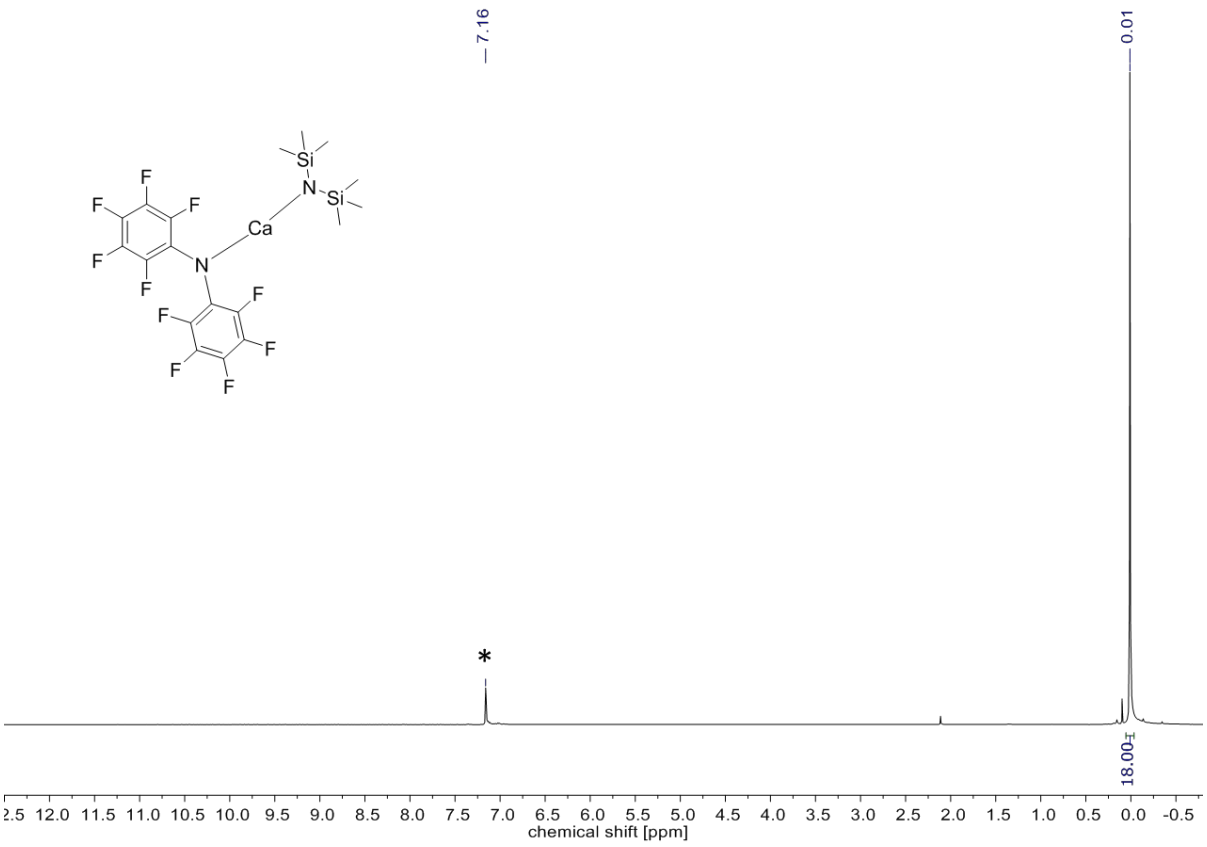

Figure S 19 ^{1}H NMR (400 MHz, C_6D_6, rt) of ($N^{F}CaN''$) .

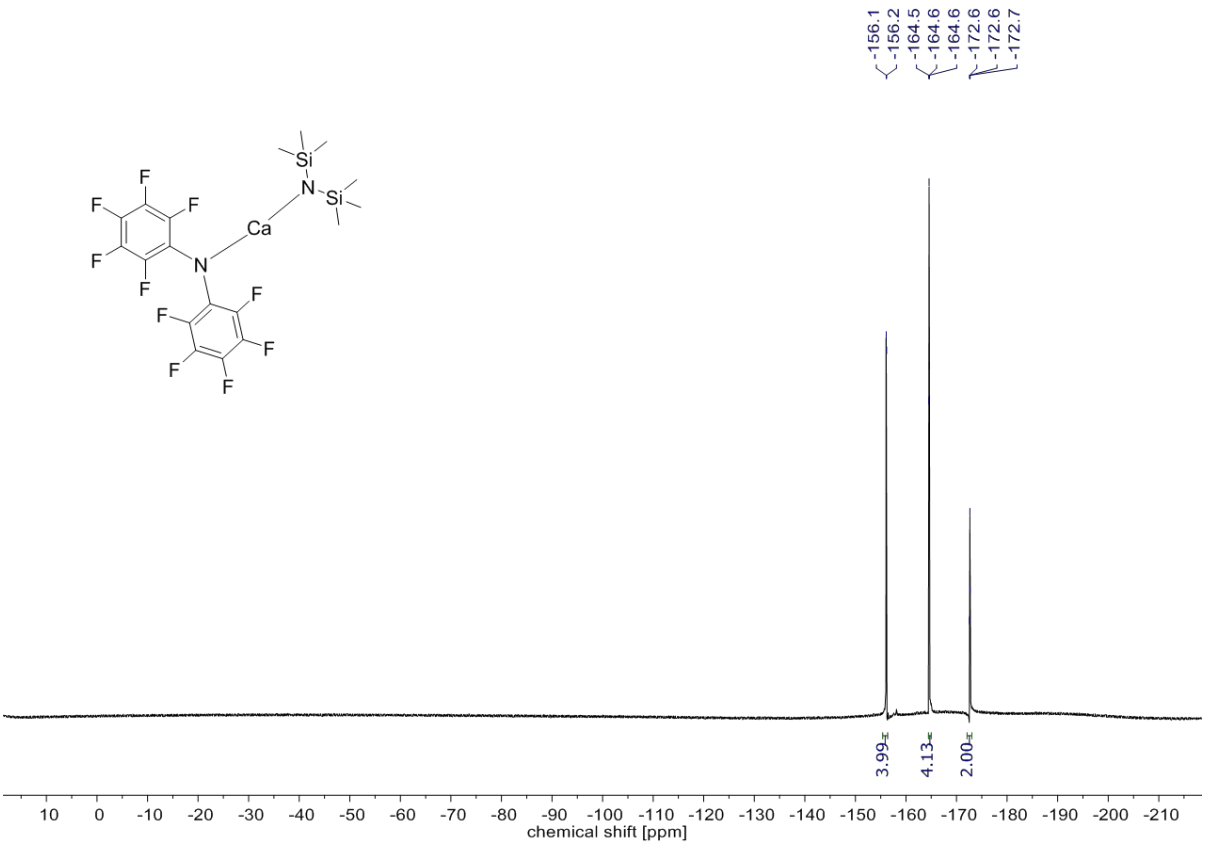

Figure S 20 $^{19}F\{^{1}H\}$ NMR (376 MHz, C_6D_6, rt) of $(N^{F}CaN'')_2$.

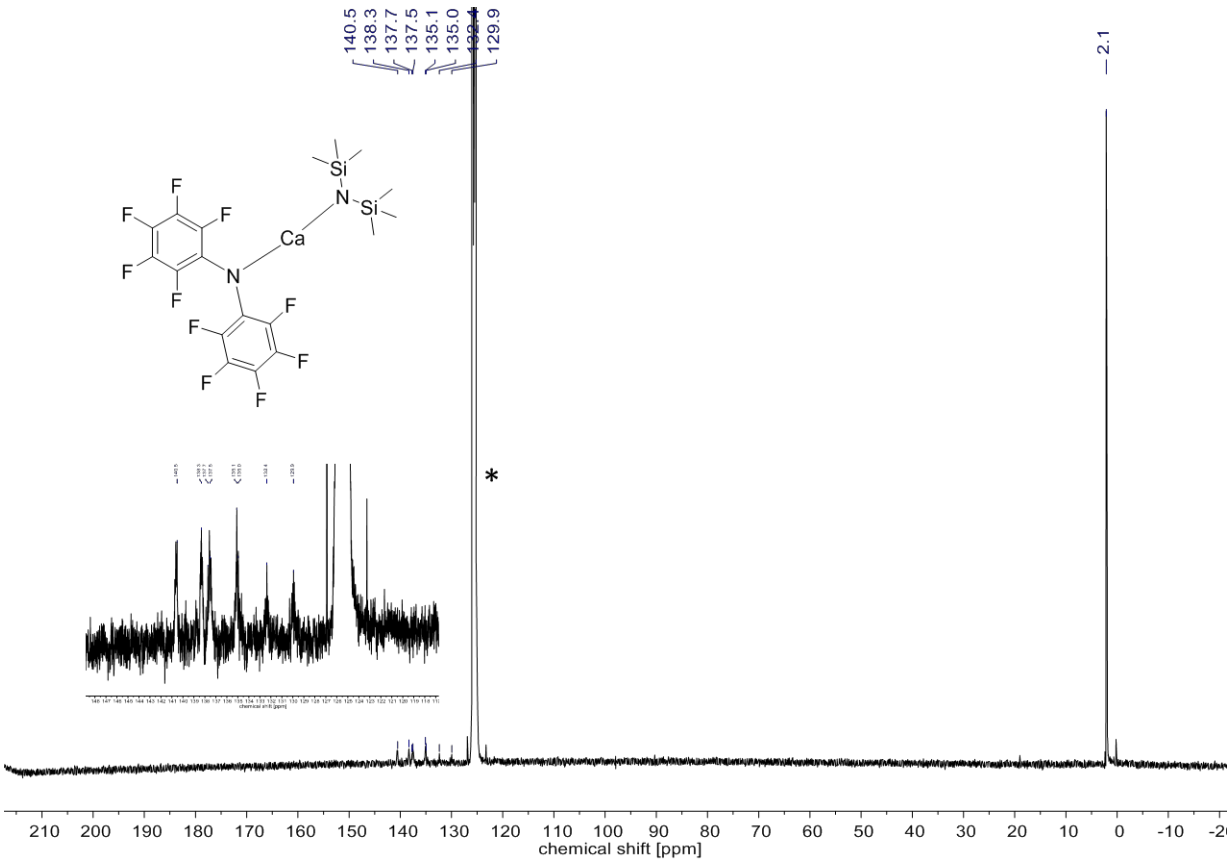

Figure S 21 ^{13}C {^{1}H} NMR (101 MHz, C_6D_6, rt) of (N^F_2CaN'') .

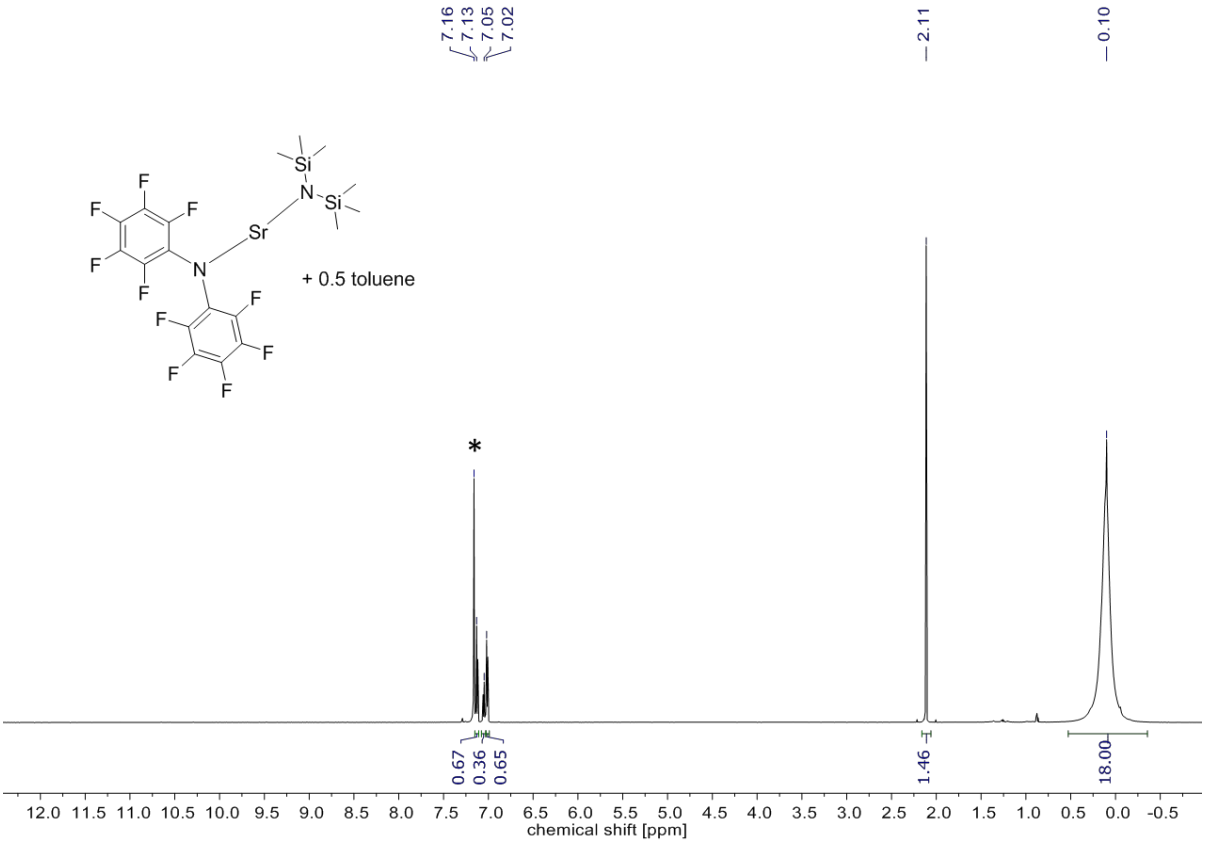

Figure S 22 ^{1}H NMR (600 MHz, C_6D_6, rt) of (N^FSrN'')$_2$, with co-crystallized toluene.

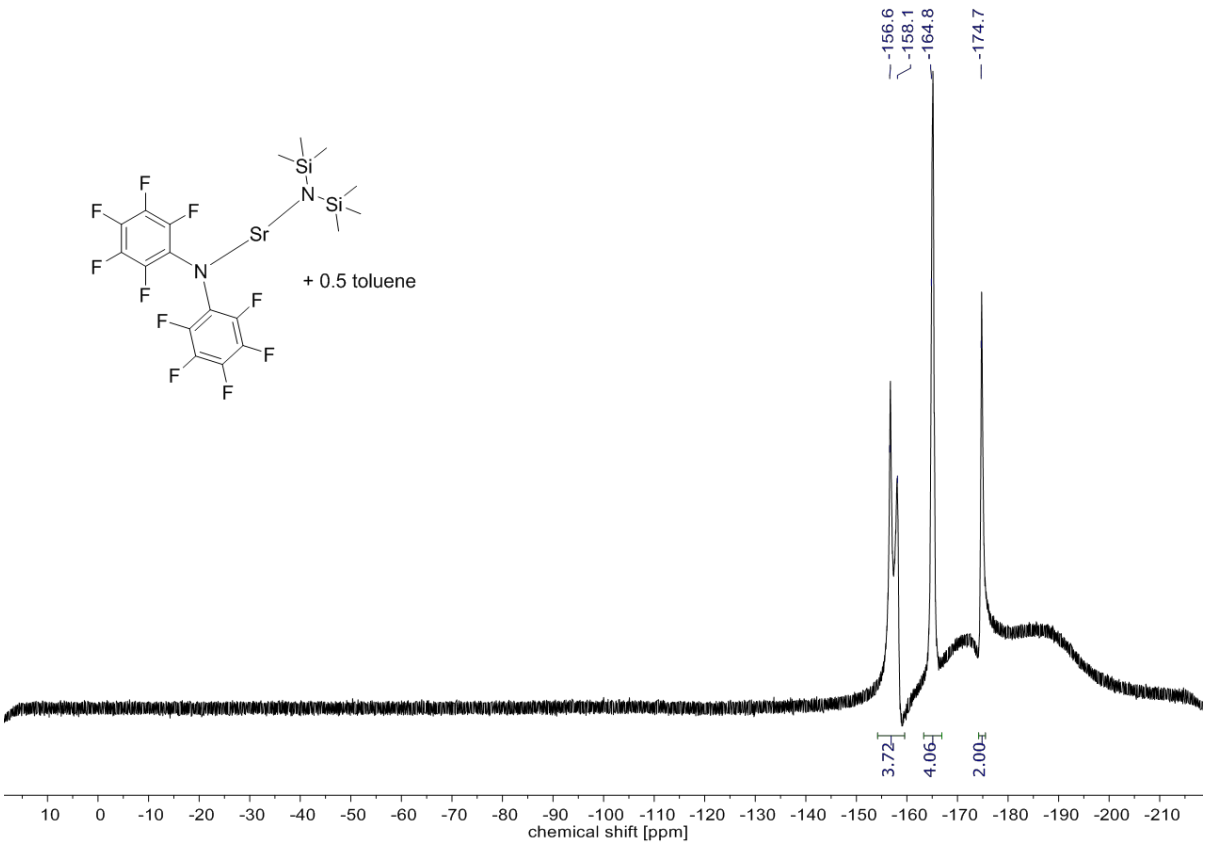

Figure S 23 $^{19}F\{^1H\}$ NMR (565 MHz, C_6D_6, rt) of $(N^FSrN'')_2$, with co-crystallized toluene.

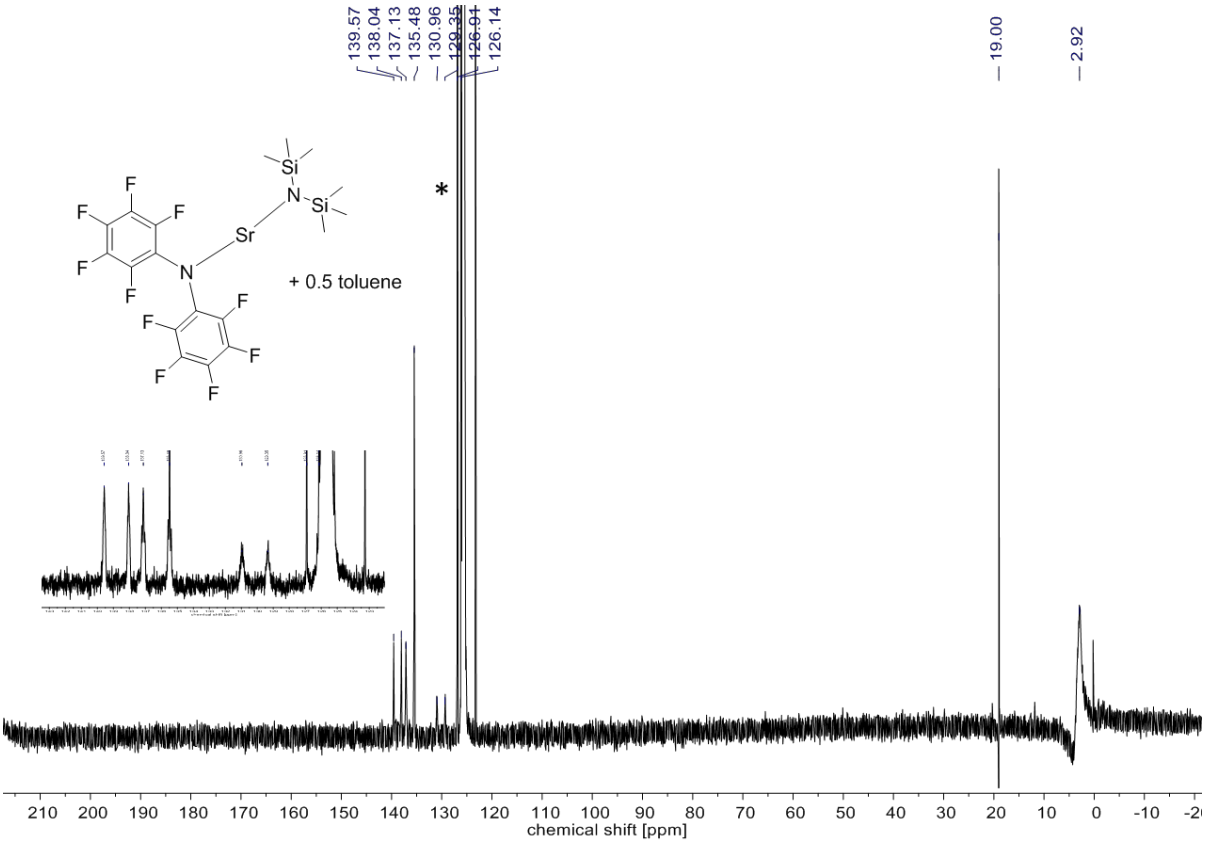

Figure S 24 $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, rt) of $(N^FSrN'')_2$, with co-crystallized toluene.

1.2 DOSY NMR measurements

Diffusion measurements were carried out at 298 K on a Bruker AVANCE NMR spectrometer operating at 600.13 MHz for proton resonance equipped with a 5 mm PABDO BB/19F-1H/D probe with Z-GRD and actively shielded gradient coil with a maximum gradient strength of 5.3500094 G/mm (at 10 A).

Parameter optimization was carried out empirically employing the pulse program ledbpgp2s1D using stimulated echo and LED (D21 = 5 ms, longitudinal eddy current delay as a Z-filter) with bipolar gradient pulses (P30) and two spoiling gradients (P19 = 600 µs) leading to values for gradient pulse length (in case of bipolar gradients "*little DELTA*"*0.5) and diffusion time (D20 = 60 ms for proton DOSY; "*big DELTA*"). Delay for gradient recovery was set to 200 µs.

The diffusion experiment was executed with variable gradients from 2% to 98% gradient strength with 32 increment values (difframp calculated with the AU-program *DOSY*). In this case the pulse program ledbpgp2s was applied for data aquiring of this pseudo-2D Experiment. Data processing was performed with the T1/T2 software package (SimFit) of TopSpin (version 3.2, Bruker Biospin) by fitting area data (integration of all peaks of interest of the same molecule) of diffusion decays. From these Stejskal-Tanner fitting curves calculated diffusion constants were obtained (with *Gamma* values for proton γ = 4258 Hz/G) and assimilated statistically.

The molecular weight was determined according to the publication "Molecular Weight Estimation of Molecules Incorporating Elements from van-der-Waals Corrected ECC-DOSY" from the group of Stalke.[1] C_6D_5H is used as internal reference; the aggregation in solution is similar for all examined compounds; based on the estimated molecular weights, an equilibrium between monomer and dimer is indicated whereby the dimeric form is largely favored. Due to overlapping of C_6D_5H and toluene signals (cocrystallized toluene) in the DOSY spectrum for $(N^FSrN'')_2$, a reliable molecular weight could not be given. The value of the hydrodynamic radius r, however, compares well to those of $(N^FMgN'')_2$ and $(N^FCaN'')_2$, implying that also the Sr complex is mainly present as a dimer.

Table S 1 Results from diffusion measurements for heteroleptic (N^F_2AeN'') complexes.

Compound	D [m^2/s]	r [Å]	MW (ECC)	MW (calc. for (NfAeN''))
$(N^FMgN'')_2$	$4.5993*10^{-10}$	6.40	928	532.8
$(N^FCaN'')_2$	$4.5993*10^{-10}$	6.15	930	548.6
$(N^FSrN'')_2$	$4.5993*10^{-10}$	6.32	-	596.1

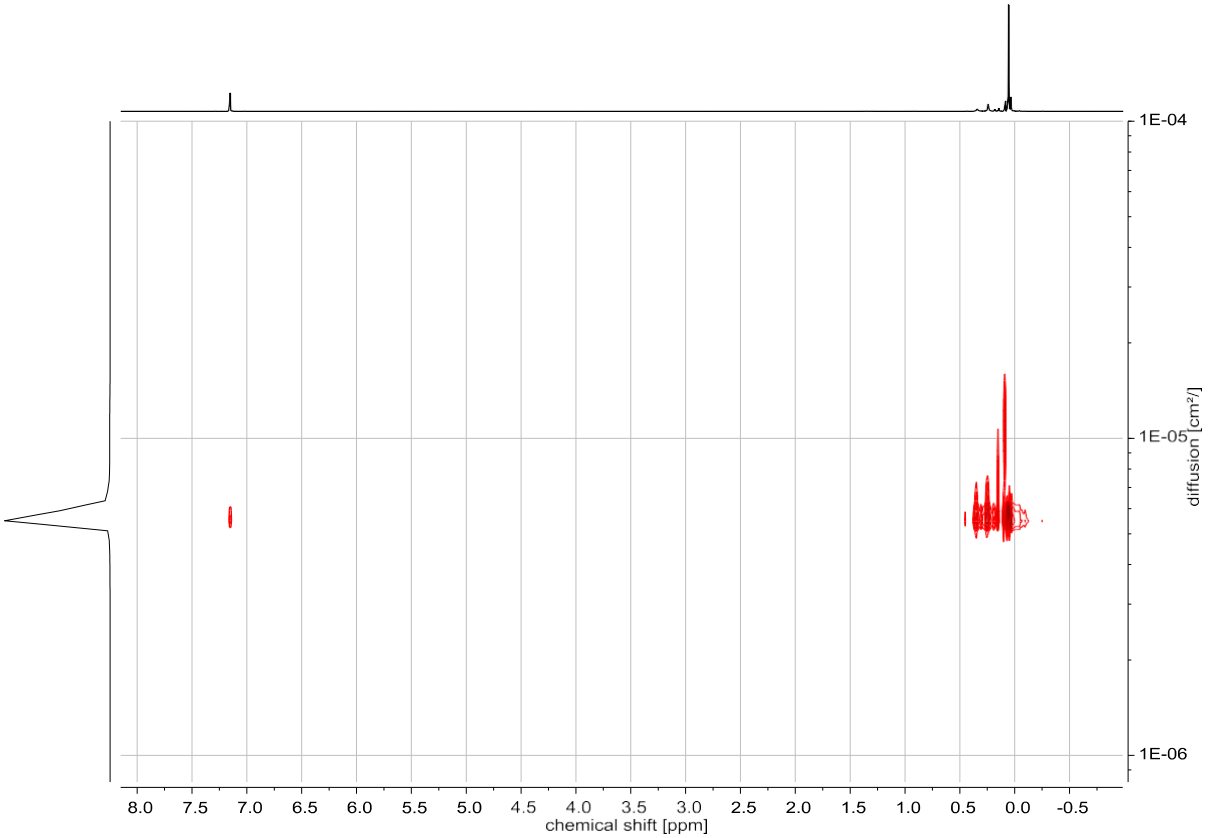

Figure S 25 ^1H DOSY NMR spectrum of $(N^FMgN'')_2$ in C_6D_6.

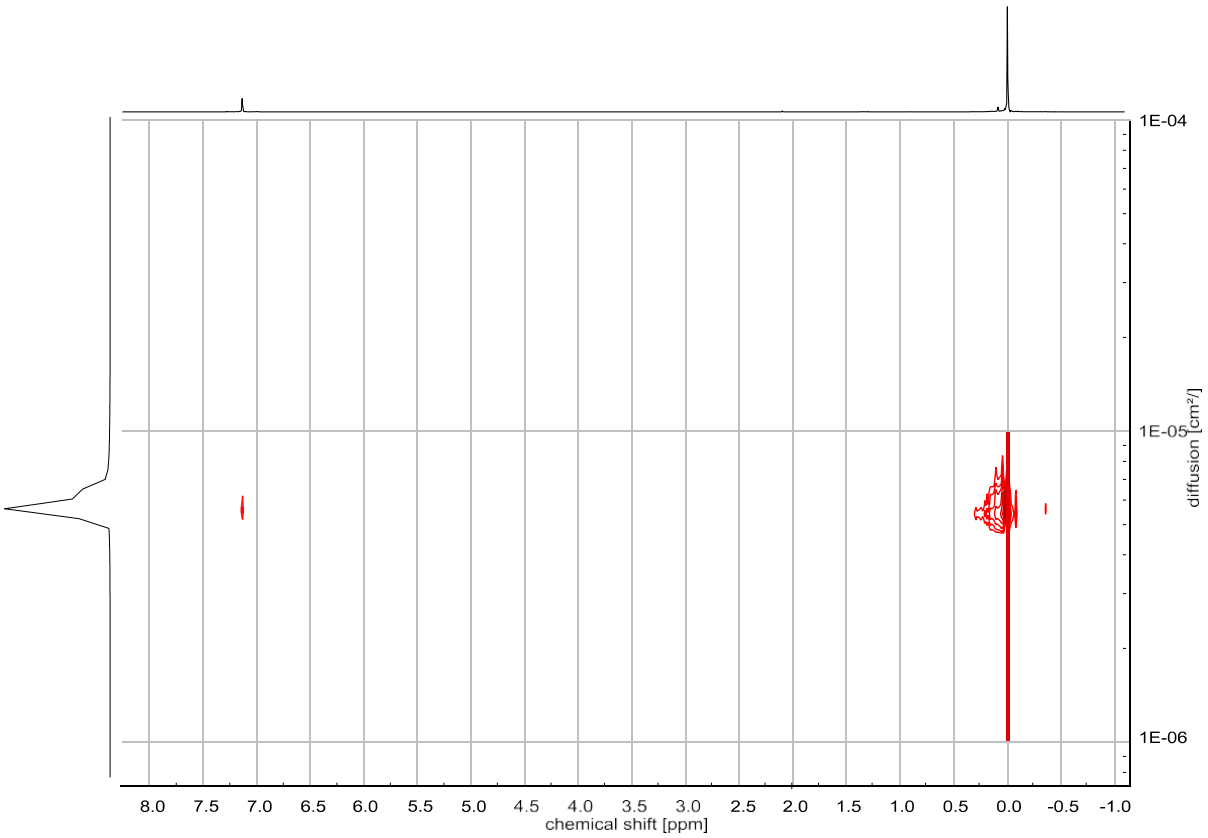

Figure S 26 ^{1}H DOSY NMR spectrum of (N^FCaN'')$_2$ in C_6D_6.

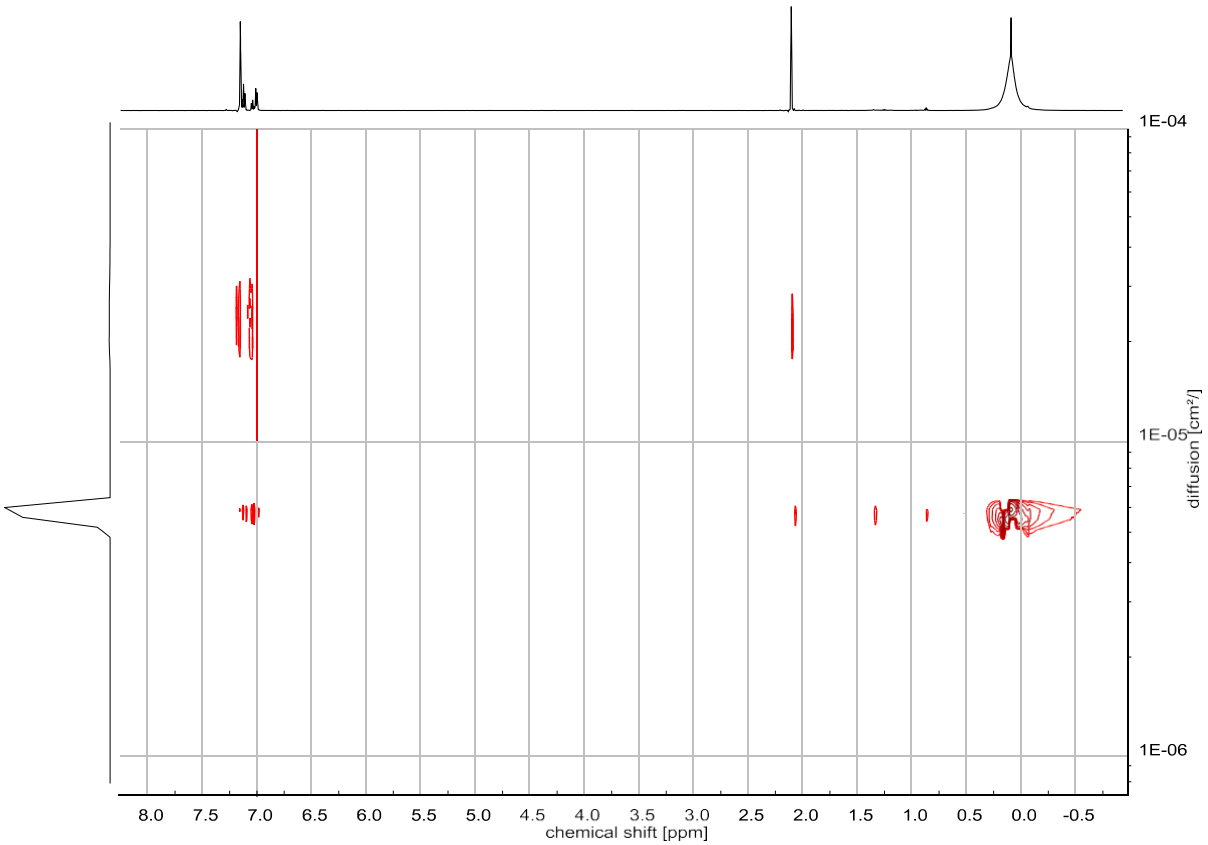

Figure S 27 ^{1}H DOSY NMR spectrum of (N^FSrN'')$_2$ with co- crystallized toluene in C_6D_6.

1.3 Lewis acidity quantification by the Gutmann-Beckett method

Lewis acidity was tested according to Gutmann and Beckett[2-3] by dissolving or suspending a portion of the respective complex in C_6D_6 (600 µL) in an NMR tube after which exactly one equivalent of Et_3PO per metal was added. If necessary the mixture was slightly heated until a clear solution was obtained. ^{31}P NMR spectra were recorded after 10 min.

Thereby the perturbation of the ^{31}P NMR chemical shift of the LEWIS base Et_3PO upon coordination to an acceptor molecule is determined. This value is converted in an acceptor number (AN) which has been calibrated using fully inert hexane (AN = 0) and the strong LEWIS acid SbF_5 (AN = 100).[4] The conversion is done according to the following formula:

$$AN = 2.21 \times (\delta(^{31}P\ NMR)_{Et_3PO} - 41.0)$$

Table S 2 ^{31}P NMR shifts of $OPEt_3$ and resulting acceptor numbers of alkaline earth metal compounds.

	^{31}P NMR shift of $OPEt_3$ (δ) *ppm+	Acceptor number Ae compound (AN)
MgN^F_2	66.8	57.0
CaN^F_2	59.2	40.2
MgN''_2	64.0	50.8
CaN''_2	61.5	45.3
MgI_2	67.6	58.8
CaI_2	58.4	38.5

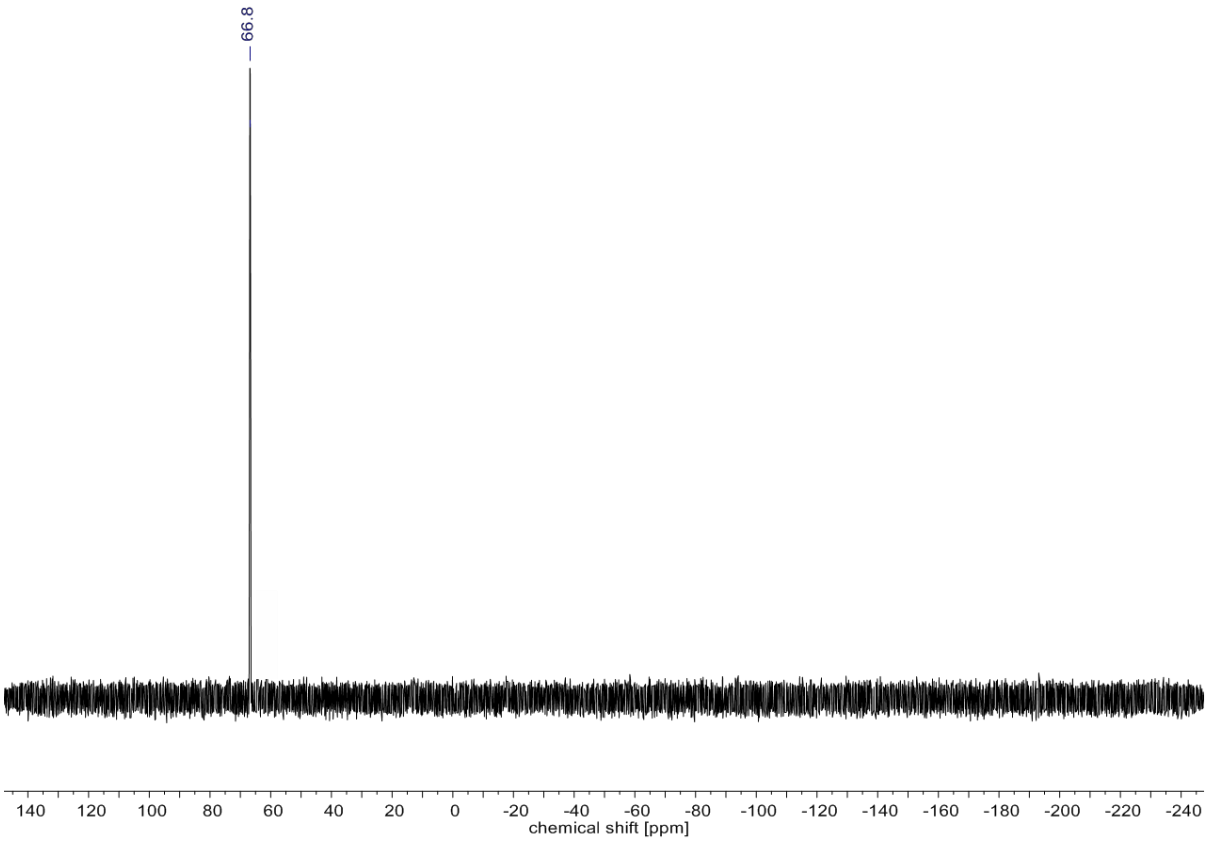

Figure S28 $^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, rt) of $OPEt_3$ with MgN^F_2

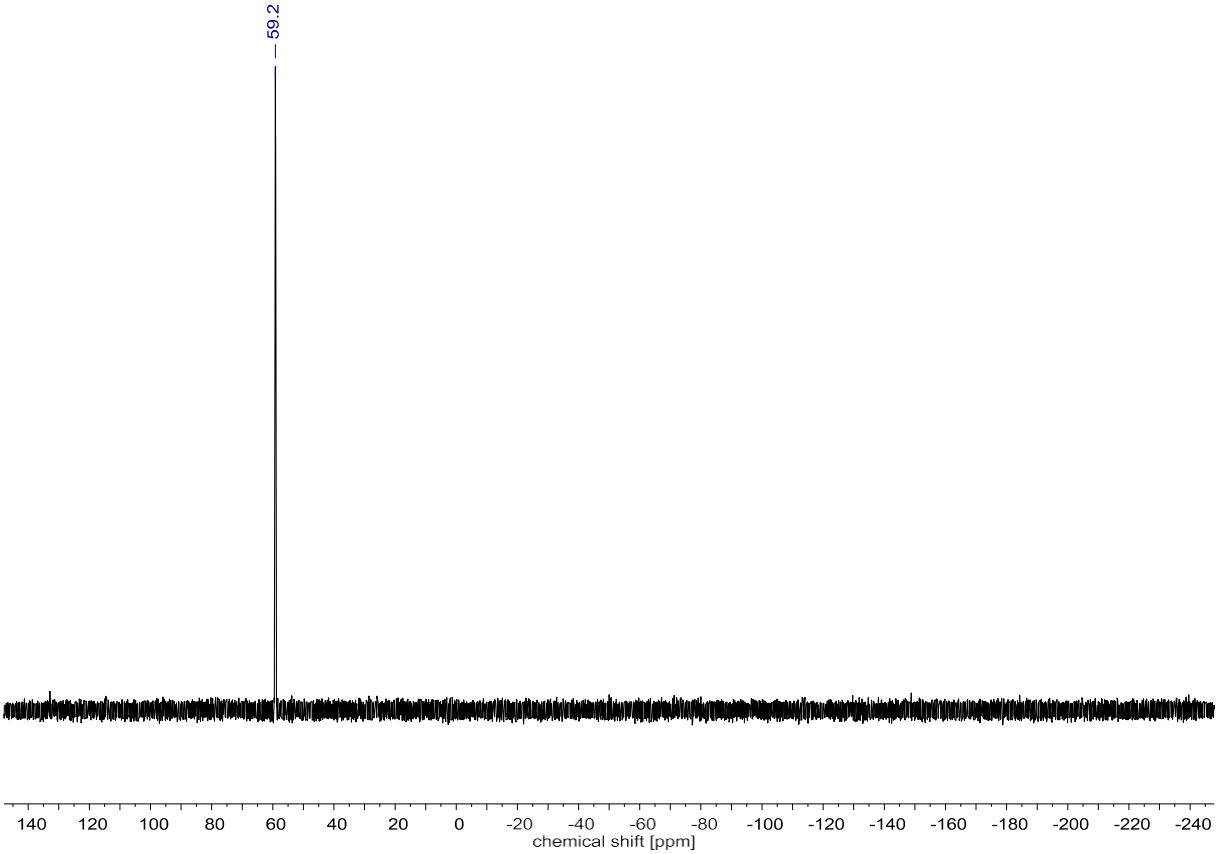

Figure S29 $^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, rt) of $OPEt_3$ with CaN^F_2

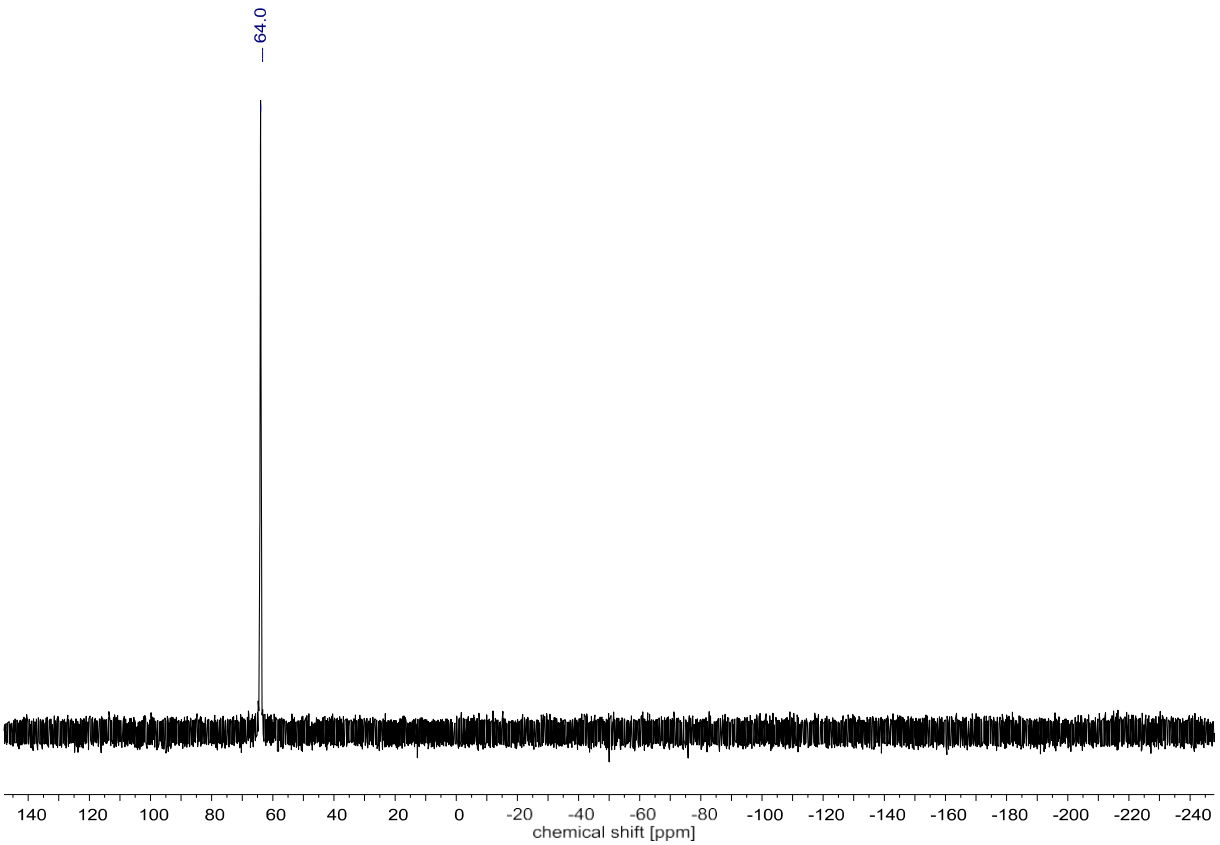

Figure S 30 $^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, rt) of $OPEt_3$ with CaN''_2.

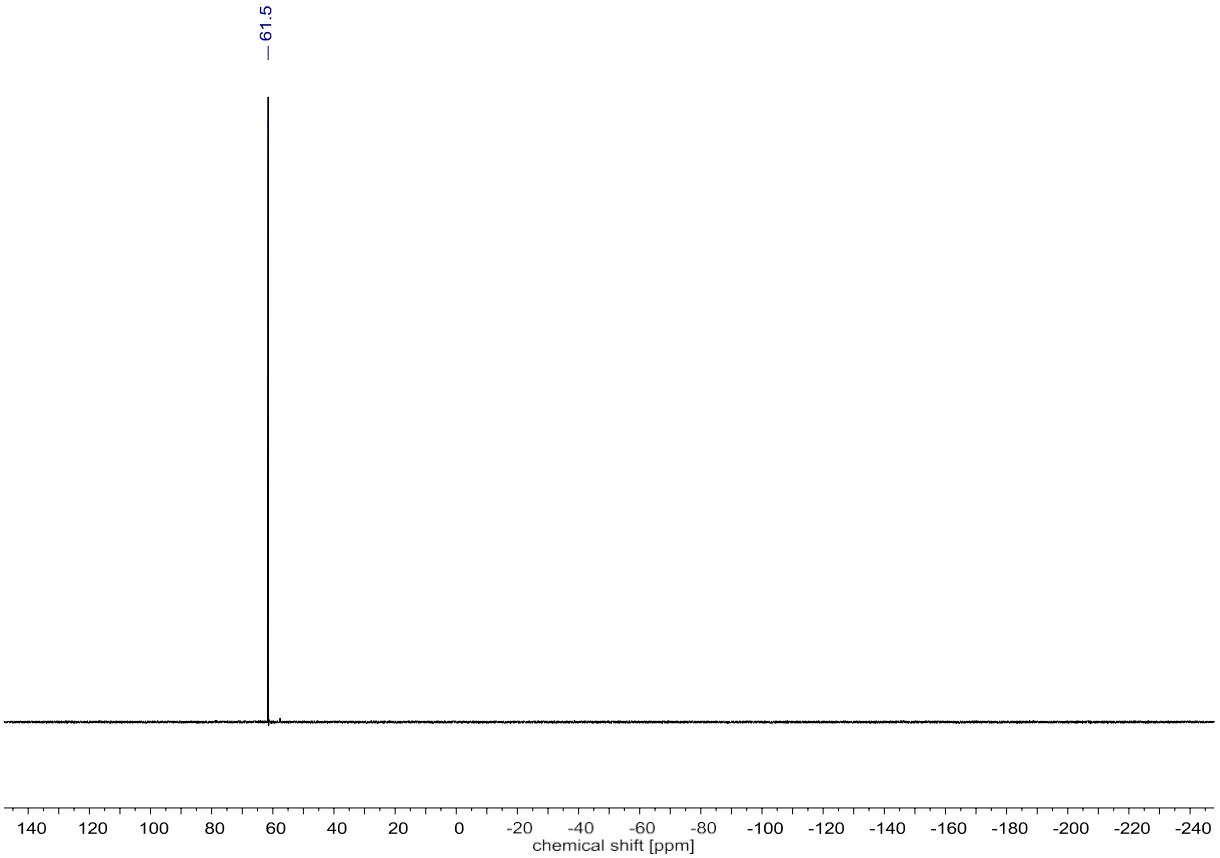

Figure S 31 $^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, rt) of $OPEt_3$ with CaN''_2.

1.4 Competition experiment between MgN^F_2 and $B(C_6F_5)_3$

Under inert conditions MgN^F_2 (16 mg; 0.022 mmol) was suspended in C_6D_6 (550 µL) and $Et_3PO{\cdot}B(C_6F_5)_3$ (14 mg; 0.022 mmol) added. Heating shortly to 60 °C resulted in a clear solution, which was examined by NMR spectroscopic methods.

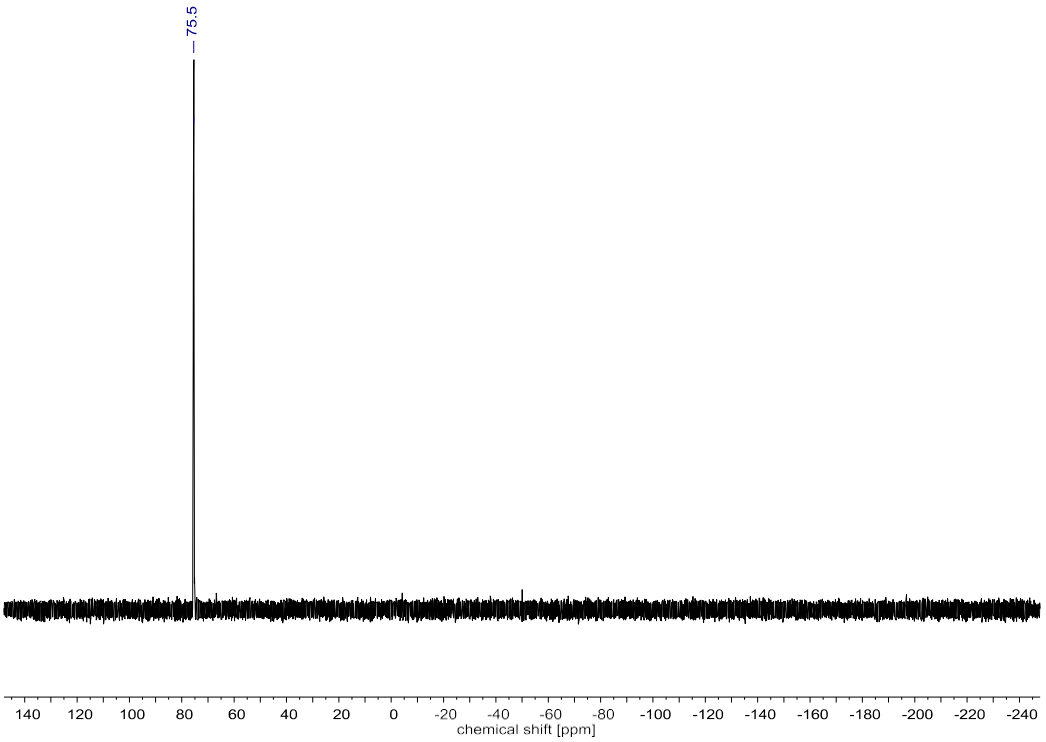

Figure S 32 $^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, rt) of $Et_3PO{\cdot}B(C_6F_5)_3$ without MgN^F_2.

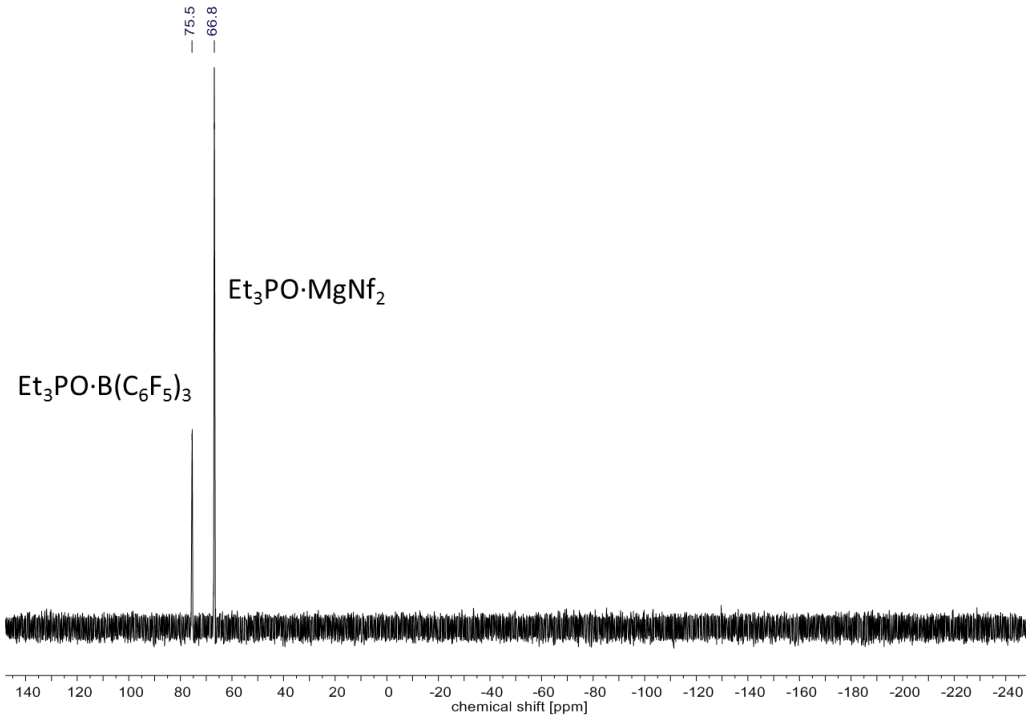

Figure S 33 $^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, rt) of $Et_3PO{\cdot}B(C_6F_5)_3$ with MgN^F_2.

1.5 Single-crystal X-ray diffraction

Magnesium bis[(decafluorodiphenyl)amide] dimer, **$(MgN^{F}_{2})_{2}$**

A colorless crystal of compound $(MgN^{F}_{2})_{2}$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100 K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v38.46)[5] software package. Using the program Olex2[6], the structure was solved by Direct Methods (ShelXT)[7] and refined by Least Squares minimization with ShelXL[8]. The hydrogen atoms have been placed on calculated positions and were refined isotropically in a riding model. Geometry calculations and graphics were done with PLATON[9]. The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1905398 contains the supplementary crystallographic data for complex $(MgN^{F}_{2})_{2}$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

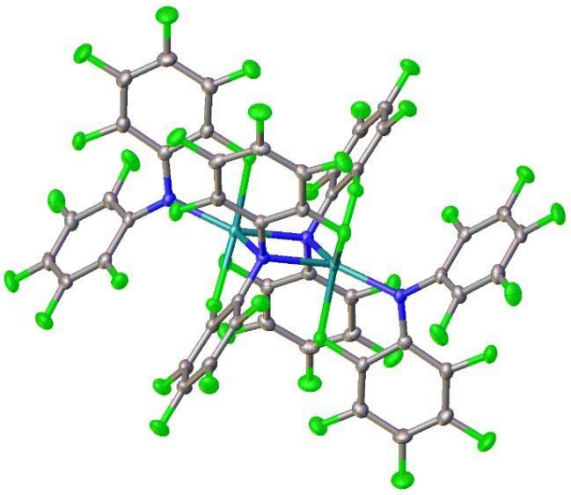

Figure S 34 ORTEP plot (50% probability) for $(MgN^{F}_{2})_{2}$.

Table S 3 Crystal data and structure refinement for $(MgN^{F}{}_{2})_{2}$.

Crystal data and structure refinement	$(MgN^{F}{}_{2})_{2}$
Identification code	hasj180309a
Empirical formula	$C_{48}F_{40}Mg_2N_4$
Formula weight	1441.14
Temperature/K	100
Crystal system	triclinic
Space group	*P*–1
a/Å	10.7838(4)
b/Å	10.8947(4)
c/Å	11.2504(4)
α/°	90.810(3)
β/°	113.380(4)
γ/°	102.982(3)
Volume/Å^3	1174.32(8)
Z	1
ρ_{calc}g/cm^3	2.038
μ/mm^{-1}	2.397
F(000)	700.0
Crystal size/mm^3	0.265 × 0.175 × 0.156
Crystal color	colorless
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.384 to 136.222
Index ranges	−12 ≤ h ≤ 12, −13 ≤ k ≤ 13, −13 ≤ l ≤ 11
Reflections collected	12778
Independent reflections	4275 [R_{int} = 0.0239, R_{sigma} = 0.0223]
Data/restraints/parameters	4275/0/424
Goodness-of-fit on F^2	1.045
Final R indexes *I>=2σ (I)+	R_1 = 0.0370, wR_2 = 0.1017
Final R indexes [all data]	R_1 = 0.0384, wR_2 = 0.1032
Largest diff. peak/hole / e Å^{-3}	0.41/−0.27

Magnesium bis[(decafluorodiphenyl)amide]·$(THF)_2$, **$MgN^F_2\cdot(THF)_2$**

A colorless crystal of compound $MgN^F_2\cdot(THF)_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100 K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v38.46)[5] software package. Using the program Olex2[6], the structure was solved by Direct Methods (ShelXT)[7] and refined by Least Squares minimization with ShelXL[8]. The hydrogen atoms have been placed on calculated positions and were refined isotropically in a riding model. Geometry calculations and graphics were done with PLATON[9]. The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1905399 contains the supplementary crystallographic data for complex $MgN^F_2\cdot(THF)_2$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

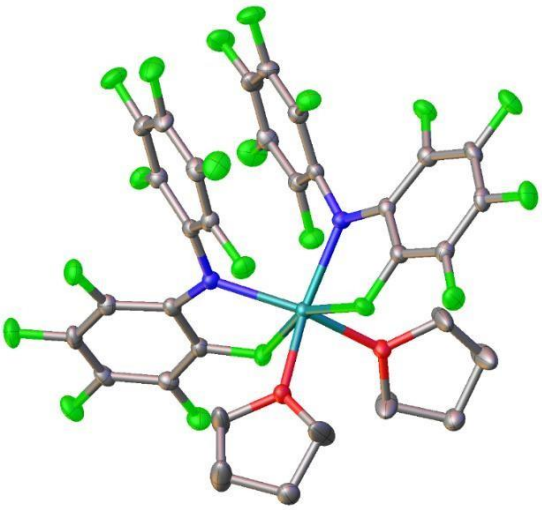

Figure S 35 ORTEP plot (50% probability) for $MgNf_2\cdot(THF)_2$.

Table S 4 Crystal data and structure refinement for $MgN^{F}_{2}\cdot(THF)_{2}$.

Crystal data and structure refinement	$MgN^{F}_{2}\cdot(THF)_{2}$
Identification code	hasj170517a
Empirical formula	$C_{32}H_{16}F_{20}MgN_2O_2$
Formula weight	864.78
Temperature/K	100
Crystal system	monoclinic
Space group	*C*2/c
a/Å	9.2647(4)
b/Å	20.2362(8)
c/Å	17.7948(7)
α/°	90
β/°	100.799(5)
γ/°	90
Volume/Å^3	3277.1(2)
Z	4
ρ_{calc}g/cm^3	1.753
μ/mm^{-1}	1.881
F(000)	1720.0
Crystal size/mm^3	0.446 × 0.39 × 0.372
Crystal color	colorless
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.74 to 136.192
Index ranges	−11 ≤ h ≤ 7, −24 ≤ k ≤ 23, −21 ≤ l ≤ 18
Reflections collected	5622
Independent reflections	2982 [R_{int} = 0.0165, R_{sigma} = 0.0208]
Data/restraints/parameters	2982/0/258
Goodness-of-fit on F^2	1.046
Final R indexes *I>=2σ (I)+	R_1 = 0.0416, wR_2 = 0.1090
Final R indexes [all data]	R_1 = 0.0440, wR_2 = 0.1112
Largest diff. peak/hole / e Å^{-3}	0.48/−0.42

Magnesium bis[(decafluorodiphenyl)amide]·$(Et_2O)_2$, **$MgN^F_2\cdot(Et_2O)_2$**

A colorless crystal of compound $MgN^F_2\cdot(Et_2O)_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 99.9(2) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v39.46)[10] software package. Using Olex2[6], the structure was solved with the ShelXT[7] structure solution program using Intrinsic Phasing and refined with the ShelXL[11] refinement package using Least Squares minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. Geometry calculations and graphics were done with PLATON[9]. The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1905400 contains the supplementary crystallographic data for complex $MgN^F_2\cdot(Et_2O)_2$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

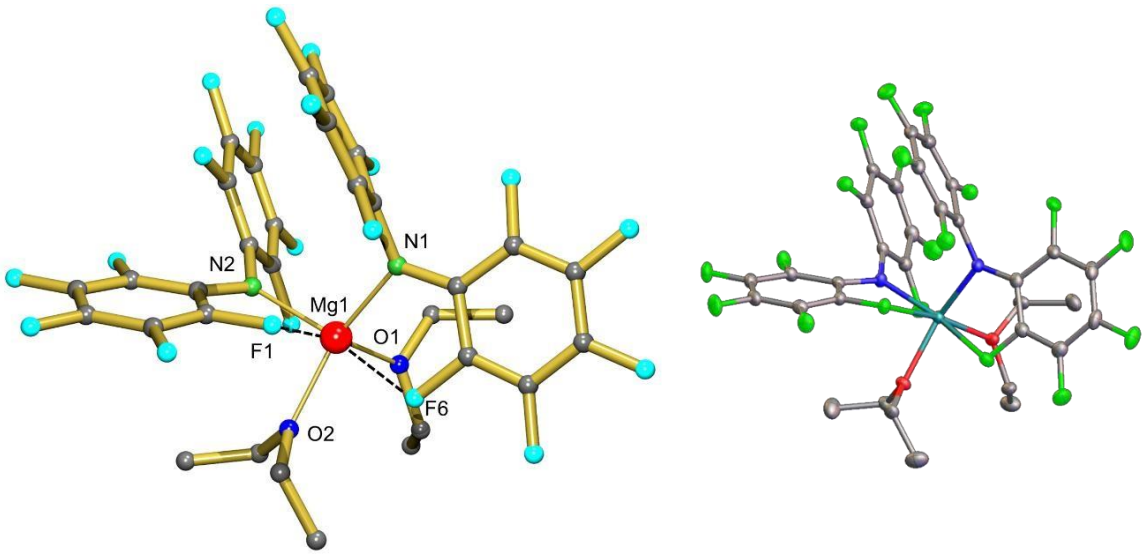

Figure S 36 Crystal structure (H omitted for clarity) and ORTEP plot (50% probability) for $MgN^F_2\cdot(Et_2O)_2$.

Table S 5 Crystal data and structure refinement for $MgNf_2·(Et_2O)_2$.

Crystal data and structure refinement	$MgN^F_2·(Et_2O)_2$
Identification code	hasj180313a
Empirical formula	$C_{32}H_{20}F_{20}MgN_2O_2$
Formula weight	868.81
Temperature/K	99.9 (2)
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	28.9330(3)
b/Å	10.43410(10)
c/Å	11.29390(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3409.51(6)
Z	4
ρ_{calc}g/cm^3	1.693
μ/mm^{-1}	1.808
F(000)	1736.0
Crystal size/mm^3	0.353 × 0.16 × 0.149
Crystal color	colorless
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.11 to 145.88
Index ranges	−35 ≤ h ≤ 35, −12 ≤ k ≤ 11, −13 ≤ l ≤ 13
Reflections collected	38139
Independent reflections	6590 [R_{int} = 0.0392, R_{sigma} = 0.0246]
Data/restraints/parameters	6590/1/518
Goodness-of-fit on F^2	1.055
Final R indexes *I>=2σ (I)+	R_1 = 0.0305, wR_2 = 0.0789
Final R indexes [all data]	R_1 = 0.0309, wR_2 = 0.0794
Largest diff. peak/hole / e Å^{-3}	0.23/−0.27

Calcium bis[(decafluorodiphenyl)amide]·$(THF)_2$, **$CaN^F_2\cdot(THF)_2$**

A colorless crystal of compound $CaN^F_2\cdot(THF)_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(1) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v38.46)[5] software package. Using the program Olex2[6], the structure was solved by Direct Methods (ShelXT)[7] and refined by Least Squares minimization with ShelXL[8]. The hydrogen atoms have been placed on calculated positions and were refined isotropically in a riding model. The THF-group was refined over two positions (ratio ~ 70:30). The THF-group was additionally modeled using Rigid Bond (RIGU) Restraints and Similar Bond Constraints (SIMU)[12]. Geometry calculations and graphics were done with PLATON[9]. The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1905401 contains the supplementary crystallographic data for complex $CaN^F_2\cdot(THF)_2$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

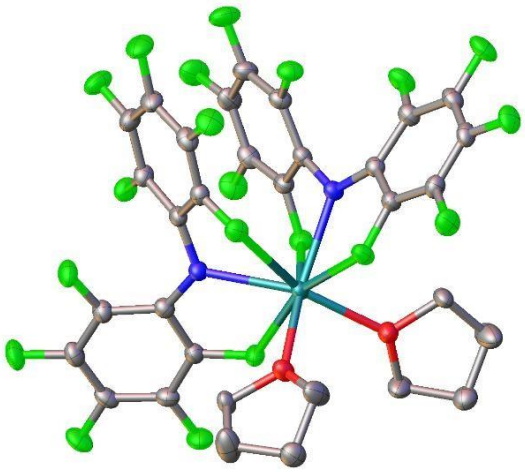

Figure S 37 ORTEP plot (50% probability) for $CaN^F_2\cdot(THF)_2$.

Table S 6 Crystal data and structure refinement for $CaN^{F}_{2}\cdot(THF)_2$.

Crystal data and structure refinement	$CaN^{F}_{2}\cdot(THF)_2$
Identification code	hasj170427a
Empirical formula	$C_{32}H_{16}CaF_{20}N_2O_2$
Formula weight	880.55
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	*C*2/c
a/Å	9.2667(2)
b/Å	20.4436(4)
c/Å	17.8288(4)
α/°	90
β/°	98.013(2)
γ/°	90
Volume/Å^3	3344.59(12)
Z	4
ρ_{calc}g/cm^3	1.749
μ/mm^{-1}	3.002
F(000)	1752.0
Crystal size/mm^3	0.353 × 0.226 × 0.124
Crystal color	colorless
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.65 to 136.23
Index ranges	−11 ≤ h ≤ 11, −24 ≤ k ≤ 16, −20 ≤ l ≤ 21
Reflections collected	9982
Independent reflections	3066 [R_{int} = 0.0204, R_{sigma} = 0.0193]
Data/restraints/parameters	3066/93/277
Goodness-of-fit on F^2	1.039
Final R indexes *I>=2σ (I)+	R_1 = 0.0317, wR_2 = 0.0821
Final R indexes [all data]	R_1 = 0.0327, wR_2 = 0.0830
Largest diff. peak/hole / e Å^{-3}	0.48/−0.38

Calcium bis[(decafluorodiphenyl)amide]·$(Et_2O)_2$, **$CaN^F_2\cdot(Et_2O)_2$**

A colorless crystal of compound $CaN^F_2\cdot(Et_2O)_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(1) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v39.46)[10] software package. Using Olex2[6], the structure was solved with the ShelXT[7] structure solution program using Intrinsic Phasing and refined with the ShelXL[11] refinement package using Least Squares minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. Geometry calculations and graphics were done with PLATON[9]. The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1905402 contains the supplementary crystallographic data for complex $CaN^F_2\cdot(Et_2O)_2$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

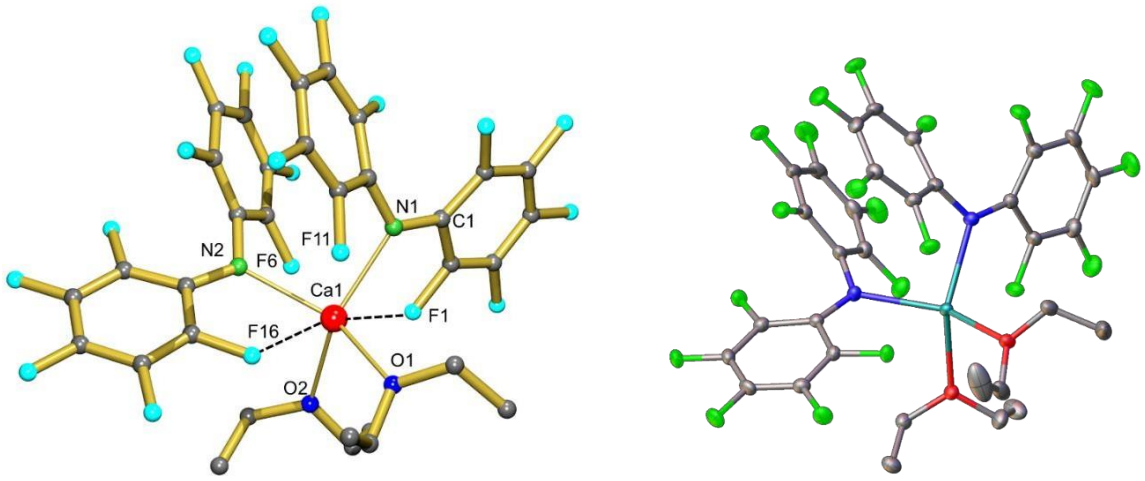

Figure S 38 Crystal structure (H omitted for clarity) and ORTEP plot (30% probability) for $CaN^F_2\cdot(Et_2O)_2$.

Table S 7 Crystal data and structure refinement for $CaNf_2·(Et_2O)_2$.

Crystal data and structure refinement	$CaN^F_2·(Et_2O)_2$
Identification code	hasj170817a
Empirical formula	$C_{32}H_{20}CaF_{20}N_2O_2$
Formula weight	884.58
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.2631(3)
b/Å	20.3100(4)
c/Å	18.1174(4)
α/°	90
β/°	91.034(2)
γ/°	90
Volume/Å^3	3407.94(15)
Z	4
ρ_{calc}g/cm^3	1.724
μ/mm^{-1}	2.947
F(000)	1768.0
Crystal size/mm^3	0.232 × 0.11 × 0.097
Crystal color	colorless
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.538 to 147.41
Index ranges	−7 ≤ h ≤ 11, −25 ≤ k ≤ 15, −21 ≤ l ≤ 21
Reflections collected	12065
Independent reflections	6645 [R_{int} = 0.0239, R_{sigma} = 0.0333]
Data/restraints/parameters	6645/0/518
Goodness-of-fit on F^2	1.025
Final R indexes *I>=2σ (I)+	R_1 = 0.0343, wR_2 = 0.0871
Final R indexes [all data]	R_1 = 0.0395, wR_2 = 0.0909
Largest diff. peak/hole / e Å^{-3}	0.42/−0.45

Strontium bis[(decafluorodiphenyl)amide]·$(THF)_2$, **$SrN^F_2\cdot(THF)_2$**

A colorless crystal of compound $SrN^F_2\cdot(THF)_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(1) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v38.46)[5] software package. Using the program Olex2[6], the structure was solved by Direct Methods (ShelXT)[7] and refined by Least Squares minimization with ShelXL[8]. The hydrogen atoms have been placed on calculated positions and were refined isotropically in a riding model. The THF-group was refined over two positions (ratio ~ 80:20). The THF-group was additionally modeled using Rigid Bond (RIGU)[12]. Geometry calculations and graphics were done with PLATON[9]. The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1905403 contains the supplementary crystallographic data for complex $SrN^F_2\cdot(THF)_2$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

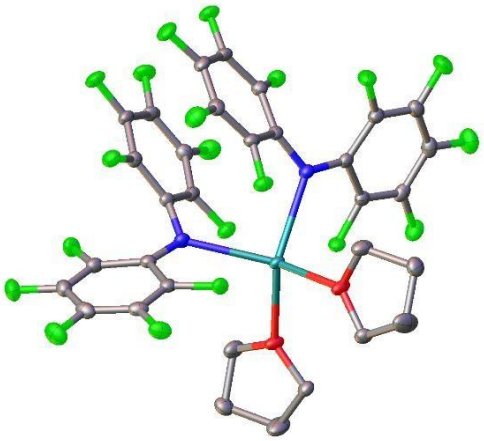

Figure S 39 ORTEP plot (50% probability) for $SrN^F_2\cdot(THF)_2$.

Table S 8 Crystal data and structure refinement for $SrNf_2·(THF)_2$.

Crystal data and structure refinement	$SrN^F_2·(THF)_2$
Identification code	hasj181130a
Empirical formula	$C_{32}H_{16}F_{20}N_2O_2Sr$
Formula weight	928.09
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	*C*2/c
a/Å	15.8863(2)
b/Å	12.46800(10)
c/Å	17.3641(2)
α/°	90
β/°	107.9700(10)
γ/°	90
Volume/Å^3	3271.54(6)
Z	4
ρ_{calc}g/cm^3	1.884
μ/mm^{-1}	3.705
F(000)	1824.0
Crystal size/mm^3	0.148 × 0.099 × 0.092
Crystal color	colorless
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.196 to 136.218
Index ranges	−19 ≤ h ≤ 17, −14 ≤ k ≤ 14, −20 ≤ l ≤ 20
Reflections collected	9108
Independent reflections	2992 [R_{int} = 0.0204, R_{sigma} = 0.0180]
Data/restraints/parameters	2992/51/278
Goodness-of-fit on F^2	1.047
Final R indexes *I>=2σ (I)+	R_1 = 0.0222, wR_2 = 0.0561
Final R indexes [all data]	R_1 = 0.0228, wR_2 = 0.0565
Largest diff. peak/hole / e Å^{-3}	0.43/−0.34

Bis[magnesium((decafluorodiphenyl)amide)(bis(trimethylsilyl)amide)], **$(N^FMgN'')_2$**

A colorless crystal of compound $(N^FMgN'')_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100 K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v38.46)[5] software package. Using the program Olex2[6], the structure was solved by Direct Methods (ShelXT)[7] and refined by Least Squares minimisation with ShelXL[8]. The hydrogen atoms have been placed on calculated positions and were refined isotropically in a riding model. Geometry calculations and graphics were done with PLATON[9]. The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1905404 contains the supplementary crystallographic data for complex $(N^FMgN'')_2$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

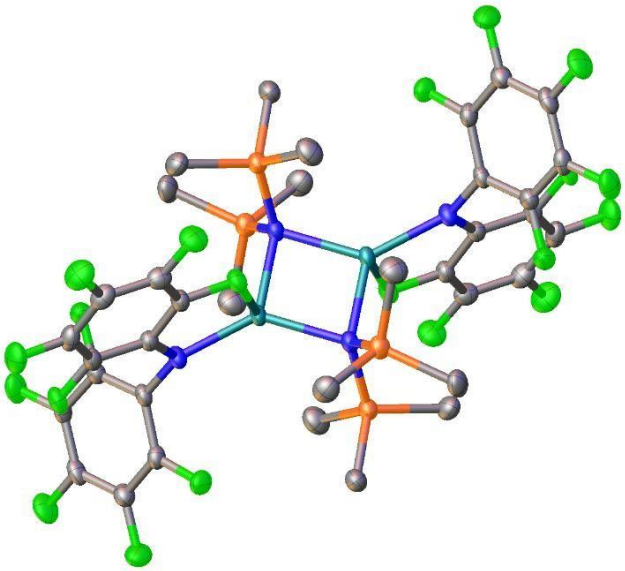

Figure S 40 ORTEP plot (50% probability) for $(N^FMgN'')_2$.

Table S 9 Crystal data and structure refinement for $(NfMgN'')_2$.

Crystal data and structure refinement	$(N^FMgN'')_2$
Identification code	hasj170503a
Empirical formula	$C_{36}H_{36}F_{20}Mg_2N_4Si_4$
Formula weight	1065.67
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.7023(3)
b/Å	15.6263(3)
c/Å	13.0643(3)
α/°	90
β/°	111.787(3)
γ/°	90
Volume/Å^3	2218.34(10)
Z	2
ρ_{calc}g/cm^3	1.595
μ/mm^{-1}	2.616
F(000)	1080.0
Crystal size/mm^3	0.242 × 0.163 × 0.147
Crystal color	colorless
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.678 to 136.19
Index ranges	−14 ≤ h ≤ 13, −11 ≤ k ≤ 18, −13 ≤ l ≤ 15
Reflections collected	7362
Independent reflections	4040 [R_{int} = 0.0225, R_{sigma} = 0.0326]
Data/restraints/parameters	4040/0/304
Goodness-of-fit on F^2	1.038
Final R indexes *I>=2σ (I)+	R_1 = 0.0366, wR_2 = 0.1001
Final R indexes [all data]	R_1 = 0.0416, wR_2 = 0.1052
Largest diff. peak/hole / e Å^{-3}	0.32/−0.37

Bis[calcium((decafluorodiphenyl)amide)(bis(trimethylsilyl)amide)], **$(N^{F}CaN'')_2$**

A colorless crystal of $(N^{F}CaN'')_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 200.0(1) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v39.46)[10] software package. Using Olex2[6], the structure was solved with the ShelXT[7] structure solution program using Intrinsic Phasing and refined with the ShelXL[11] refinement package using Least Squares minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. Geometry calculations and graphics were done with PLATON[9]. The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1905405 contains the supplementary crystallographic data for complex $(N^{F}CaN'')_2$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

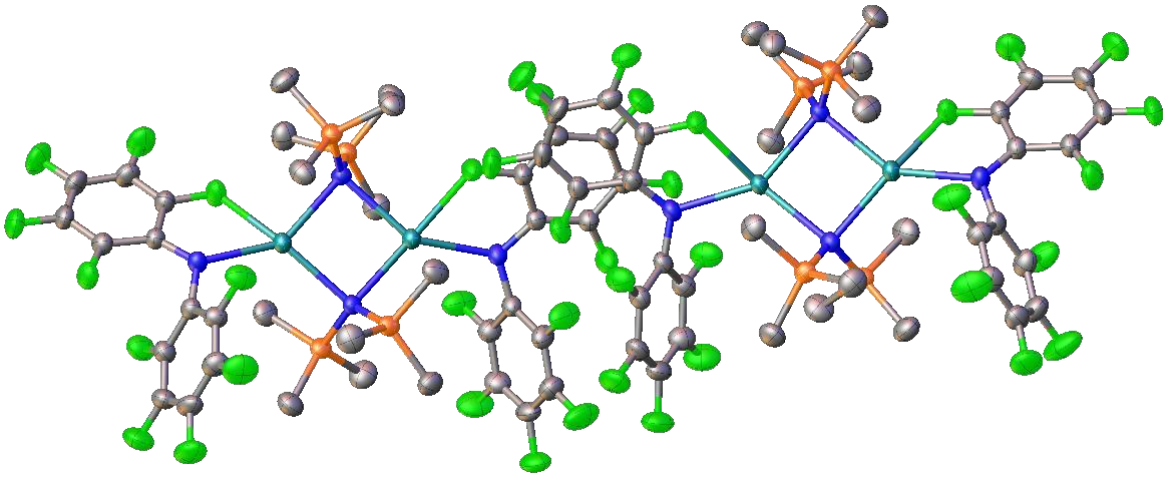

Figure S 41 ORTEP plot (50% probability) for $(NfCaN'')_2$.

Table S 10 Crystal data and structure refinement for $(N^F CaN'')_2$.

Crystal data and structure refinement	$(NfCaN'')_2$
Identification code	hasj180921b
Empirical formula	$C_{36}H_{36}Ca_2F_{20}N_4Si_4$
Formula weight	1097.21
Temperature/K	200.0(1)
Crystal system	triclinic
Space group	*P*−1
a/Å	8.8864(2)
b/Å	24.4425(6)
c/Å	24.5767(7)
α/°	63.347(3)
β/°	83.970(2)
γ/°	89.760(2)
Volume/Å^3	4739.0(2)
Z	4
ρ_{calc}g/cm^3	1.538
μ/mm^{-1}	4.085
F(000)	2224.0
Crystal size/mm^3	0.327 × 0.121 × 0.077
Crystal color	colorless
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.9 to 147.808
Index ranges	−8 ≤ h ≤ 10, −30 ≤ k ≤ 30, −25 ≤ l ≤ 30
Reflections collected	30487
Independent reflections	18418 [R_{int} = 0.0308, R_{sigma} = 0.0492]
Data/restraints/parameters	18418/0/1213
Goodness-of-fit on F^2	1.024
Final R indexes *I>=2σ (I)+	R_1 = 0.0434, wR_2 = 0.1099
Final R indexes [all data]	R_1 = 0.0573, wR_2 = 0.1201
Largest diff. peak/hole / e Å^{-3}	0.29/−0.60

Bis[strontium((decafluorodiphenyl)amide)(bis(trimethylsilyl)amide)], **$(N^FSrN'')_2$**

A colorless crystal of compound $(N^FSrN'')_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(1) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v39.46)[10] software package. Using Olex2[6], the structure was solved with the ShelXT[7] structure solution program using Intrinsic Phasing and refined with the ShelXL[11] refinement package using Least Squares minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. Two benzene molecules with occupancies of 1:1 were additionally modeled using Rigid Bond (RIGU) Restraints and additionally similarity restraints (SIMU)[12]; two disordered benzene molecules were found on a symmetry element and were refined with large displacement factors. Geometry calculations and graphics were done with PLATON[9]. The crystal structure data has been deposited with the Cambridge Crystallographic Data Centre. CCDC 1905406 contains the supplementary crystallographic data for complex $(N^FSrN'')_2$. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

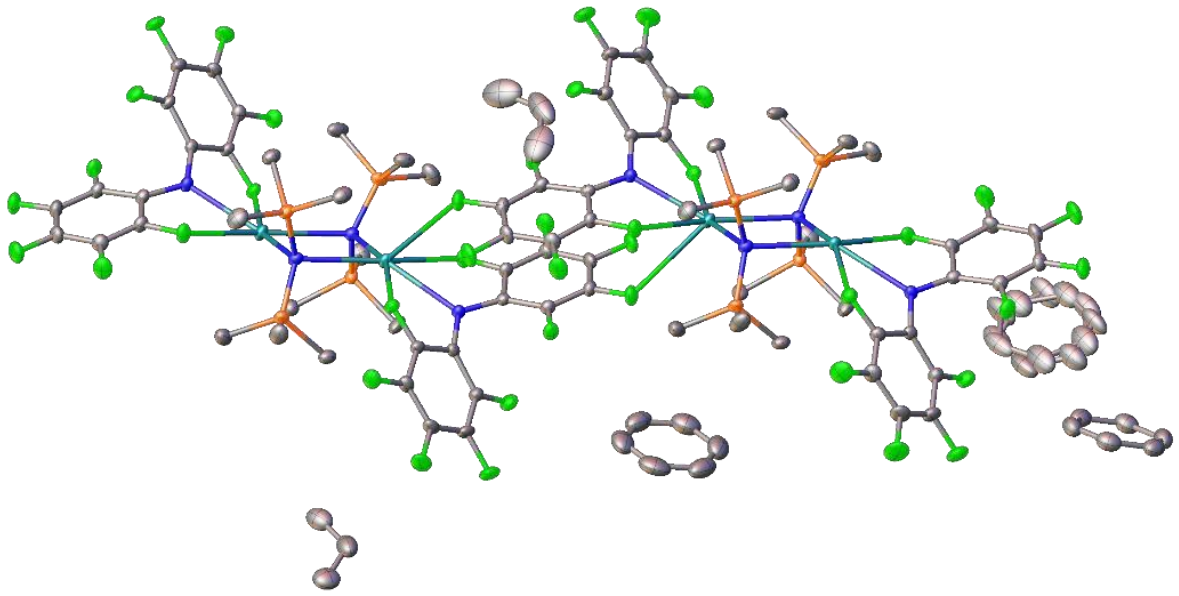

Figure S 42 ORTEP plot (50% probability) for $(N^FSrN'')_2$.

Table S 11 Crystal data and structure refinement for $(N^FSrN'')_2$.

Crystal data and structure refinement	$(N^FSrN'')_2$
Identification code	hasj180302a
Empirical formula	$C_{48}H_{48}F_{20}N_4Si_4Sr_2$
Formula weight	1348.50
Temperature/K	100.0(1)
Crystal system	triclinic
Space group	*P*–1
a/Å	12.5188(2)
b/Å	20.5028(3)
c/Å	23.2272(2)
α/°	99.6880(10)
β/°	99.7680(10)
γ/°	102.2650(10)
Volume/Å^3	5610.49(13)
Z	4
ρ_{calc}g/cm^3	1.596
μ/mm^{-1}	4.269
F(000)	2704.0
Crystal size/mm^3	0.2785 × 0.2206 × 0.1705
Crystal color	colorless
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.6 to 145.902
Index ranges	−15 ≤ h ≤ 15, −25 ≤ k ≤ 24, −28 ≤ l ≤ 28
Reflections collected	104506
Independent reflections	21992 [R_{int} = 0.0422, R_{sigma} = 0.0252]
Data/restraints/parameters	21992/258/1460
Goodness-of-fit on F^2	1.067
Final R indexes *I>=2σ (I)+	R_1 = 0.0439, wR_2 = 0.1203
Final R indexes [all data]	R_1 = 0.0504, wR_2 = 0.1269
Largest diff. peak/hole / e Å^{-3}	1.34/−0.57

2 DFT calculations

All calculations were carried out using Gaussian 16A.[13] All methods were used as implemented. Structures were optimized on a B3PW91/6-311+G** level of theory,[14-17] except for iodine-containing complexes. The latter were optimized on the B3PW91/def2tzvpp level of theory,[18] which includes pseudopotentials for iodide. All optimized structures were determined to be true minima by frequency calculation (NIMAG=0). Charges were calculated using the Natural Bond Orbital analysis.[19] Structures were drawn and evaluated using Molecule.[20] Topological analysis was carried out according to Bader using the Program AIMAll17 with the wave function obtained from the optimization.[21-22]

XYZ-Coordinates

	102		
$(N^{F}MgN'')_2$			
Si	-0.583365	1.882027	2.321285
Si	0.156375	-0.947023	2.713506
Mg	1.402342	0.269817	0.019409
F	2.021386	2.342312	-0.092868
F	4.257932	-1.101384	2.523417
F	6.396663	0.565309	0.297329
F	3.060523	4.838676	-0.185787
F	6.251296	-4.663699	0.210808
F	4.341321	-1.112379	-2.190346
F	7.386399	3.016032	0.195207
F	5.552793	-3.462412	2.548127
F	5.640846	-3.473690	-2.157783
F	5.785640	5.208107	-0.041728
N	3.467314	0.146583	0.141993
N	-0.136977	0.346914	1.502838
C	4.213418	-1.046753	0.164383
C	4.143402	1.340006	0.106509
C	3.388697	2.515206	-0.014701
C	5.530972	1.582536	0.175065
C	4.563980	-1.680033	1.359896
C	3.885261	3.800111	-0.066933
C	4.606993	-1.687171	-1.013759
C	5.258139	3.985198	0.003537
C	5.604770	-3.502924	0.195706
C	5.288067	-2.895706	-1.011603
C	5.243013	-2.889437	1.387146
C	6.066772	2.862620	0.123974
C	-1.412832	-1.691005	3.451886

H	-1.831618	-1.081290	4.253914
H	-1.163670	-2.668490	3.880158
H	-2.202746	-1.852431	2.714786
C	1.259860	-0.382970	4.135634
H	2.246490	-0.070957	3.783732
H	1.411477	-1.241673	4.799666
H	0.842021	0.422445	4.742533
C	-1.730279	1.628066	3.800658
H	-2.646857	1.098042	3.528167
H	-2.022429	2.623307	4.154659
H	-1.277715	1.109909	4.647830
C	0.904477	2.880527	2.907618
H	1.636721	2.281117	3.451932
H	0.555622	3.666992	3.586099
H	1.416890	3.377113	2.081117
C	1.077796	-2.388750	1.920219
H	0.419642	-3.044209	1.350230
H	1.496495	-2.987483	2.736496
H	1.929538	-2.123720	1.285381
C	-1.570124	3.019386	1.186784
H	-0.967101	3.515562	0.428134
H	-1.989838	3.807165	1.822460
H	-2.428605	2.547334	0.696541
Si	0.224669	-1.642991	-2.523710
Si	0.132144	1.290866	-2.826530
Mg	-1.413948	-0.062633	-0.152043
F	-1.811858	-2.179751	0.213714
F	-3.789508	1.631818	-2.314754
F	-6.313348	-0.925565	-0.542894
F	-2.581295	-4.765492	0.420578
F	-6.723498	4.327062	0.170905
F	-5.013936	0.385382	2.066951
F	-7.048103	-3.460482	-0.302560
F	-5.316478	3.838618	-2.108956
F	-6.568930	2.579070	2.249958
F	-5.238918	-5.439109	0.176041
N	-3.481117	-0.169491	-0.218878
N	0.109161	-0.072408	-1.647797
C	-4.343017	0.932260	-0.128829
C	-4.019534	-1.429689	-0.118418
C	-3.147613	-2.503663	0.104074
C	-5.363410	-1.829188	-0.266018
C	-4.454370	1.852476	-1.173931
C	-3.505291	-3.831794	0.205137
C	-5.081649	1.220645	1.025316
C	-4.844453	-4.170407	0.079941
C	-5.964721	3.239738	0.073326
C	-5.885399	2.344166	1.132317
C	-5.242024	2.991624	-1.084514
C	-5.761808	-3.154473	-0.157413
C	1.878969	1.674113	-3.429192
H	2.289798	0.899591	-4.077878

H	1.852818	2.606687	-4.004062
H	2.588631	1.822647	-2.610385
C	-0.981338	1.019336	-4.325865
H	-2.026668	0.895748	-4.031878
H	-0.923867	1.924293	-4.941504
H	-0.704032	0.179343	-4.964074
C	1.387658	-1.638776	-4.010421
H	2.420926	-1.436043	-3.720232
H	1.361632	-2.651932	-4.428436
H	1.116718	-0.955036	-4.815711
C	-1.466270	-2.215443	-3.136087
H	-1.872389	-1.558479	-3.907607
H	-1.363189	-3.214161	-3.575125
H	-2.217267	-2.292419	-2.345298
C	-0.505317	2.896250	-2.079248
H	0.142055	3.309401	-1.304958
H	-0.524327	3.627852	-2.895073
H	-1.527499	2.835573	-1.700196
C	0.909594	-3.025710	-1.443183
H	0.222118	-3.364868	-0.669020
H	1.086752	-3.880278	-2.105874
H	1.871891	-2.792394	-0.978051

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$N^{F}MgN$”

Si	3.741803	0.724700	1.419460
Si	3.742257	-0.721262	-1.419889
Mg	1.150764	0.001858	-0.001170
F	0.454407	2.027727	-1.003733
F	0.456881	-2.025366	1.005457
F	-3.472367	0.625314	1.188437
F	-0.552903	4.557025	-1.176884
F	-3.047113	-5.097945	0.200246
F	-3.470255	-0.629941	-1.190280
F	-4.476744	3.097455	0.976928
F	-0.546734	-4.555983	1.179399
F	-4.471279	-3.103652	-0.978021
F	-3.054666	5.094737	-0.199219
N	-0.875522	-0.000041	-0.000350
N	3.087772	0.002586	-0.000778
C	-1.524243	-1.216268	0.033511
C	-1.526180	1.215106	-0.033547
C	-0.815173	2.295865	-0.570298
C	-2.770108	1.547793	0.523060
C	-0.811954	-2.295550	0.571365
C	-1.289823	3.589626	-0.639476
C	-2.767291	-1.551099	-0.523867
C	-2.556269	3.862411	-0.136902
C	-2.550387	-3.864961	0.137593
C	-3.279682	-2.839183	-0.450492
C	-1.284749	-3.590038	0.640913
C	-3.284374	2.835215	0.450072

C	4.726014	0.471055	-2.499264
H	5.628121	0.817541	-1.985032
H	5.043991	-0.006235	-3.432533
H	4.134742	1.355352	-2.756302
C	4.809538	-2.238053	-1.082364
H	4.269628	-2.980683	-0.486975
H	5.126576	-2.717326	-2.014897
H	5.715215	-1.968655	-0.529548
C	4.807705	2.242868	1.083669
H	4.267123	2.985555	0.488959
H	5.124218	2.721552	2.016686
H	5.713666	1.974868	0.530626
C	4.727077	-0.468219	2.496763
H	5.629734	-0.812344	1.981910
H	5.044360	0.007848	3.430886
H	4.137138	-1.353870	2.752158
C	2.220676	-1.290455	-2.422024
H	1.560528	-0.457878	-2.706024
H	2.520120	-1.757683	-3.366065
H	1.628598	-2.050629	-1.892939
C	2.219969	1.291143	2.422679
H	1.561163	0.457400	2.706267
H	2.519282	1.758119	3.366891
H	1.626537	2.050939	1.894555

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N^{F}MgN”-F(-)

Si	-3.984150	1.297553	-0.859166
Si	-2.736817	0.535974	1.808843
Mg	-0.860196	1.182310	-0.792196
F	0.776152	2.525350	0.543299
F	-0.919783	-1.334996	-1.893894
F	3.450605	-1.031481	-1.057475
F	2.985673	4.067067	0.778112
F	0.167447	-5.510561	0.004588
F	2.339962	-1.623317	1.517266
F	5.630224	0.486938	-0.766393
F	-1.299488	-4.006634	-1.744260
F	1.992791	-4.278176	1.614442
F	5.447532	3.053688	0.142327
N	0.829954	-0.003993	-0.330481
N	-2.622695	0.958284	0.147164
C	0.753707	-1.370723	-0.233242
C	2.018279	0.664716	-0.199025
C	1.982295	2.003814	0.230448
C	3.300427	0.202032	-0.547621
C	-0.190763	-2.052778	-1.020451
C	3.098053	2.807806	0.345398
C	1.465320	-2.183272	0.667601
C	4.348400	2.295644	0.024960
C	0.349671	-4.185483	-0.069328
C	1.283420	-3.555067	0.739432

C	-0.398268	-3.417806	-0.951783
C	4.436149	0.987019	-0.424288
C	-3.997722	1.577691	2.780430
H	-5.016274	1.470526	2.394006
H	-4.012481	1.277977	3.835096
H	-3.737300	2.640542	2.737950
C	-3.219247	-1.280649	2.083566
H	-2.492315	-1.948729	1.609616
H	-3.256504	-1.529356	3.150889
H	-4.199867	-1.503886	1.652077
C	-5.478602	0.165066	-0.538737
H	-5.867270	0.253917	0.480791
H	-6.295899	0.416959	-1.225018
H	-5.215330	-0.884625	-0.705406
C	-3.534445	1.068924	-2.681834
H	-3.317405	0.019712	-2.909715
H	-4.370551	1.379316	-3.319595
H	-2.658764	1.665738	-2.962675
C	-1.088464	0.781353	2.708735
H	-0.786300	1.833286	2.716394
H	-1.180698	0.454264	3.750927
H	-0.276923	0.205549	2.253847
C	-4.604228	3.081235	-0.667705
H	-3.804131	3.786014	-0.917383
H	-5.453298	3.286943	-1.330494
H	-4.920754	3.287459	0.359777
F	-0.495198	2.298136	-2.199827

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$MgN^{F}_{2}\cdot(THF)_{2}$

Mg	-0.000055	1.371620	0.000049
F	2.196730	-2.634991	-0.085856
F	1.936912	1.731092	-1.270597
F	3.859255	-1.231825	1.867382
F	-0.095927	0.194003	2.922121
F	4.401904	2.304535	-2.230945
F	6.614285	1.065478	-1.166950
F	1.372744	-4.774638	1.310397
F	6.269862	-0.699082	0.881743
F	-0.970100	-1.961783	4.272658
F	-0.230765	-4.471406	3.492150
O	-0.606909	2.936784	-1.332280
N	1.471557	0.008748	0.672160
C	3.028277	1.092981	-0.750914
C	1.100965	-1.133517	1.377025
C	2.772434	0.169509	0.273693
C	5.392207	0.788352	-0.709418
C	3.940739	-0.402497	0.817323
C	4.274695	1.410797	-1.248236
C	1.438234	-2.441503	1.000208
C	0.193121	-3.405298	2.817098
C	1.013711	-3.555249	1.707129

C	0.269144	-1.030661	2.497384
C	5.207661	-0.116835	0.327708
C	-0.185736	-2.129545	3.207479
C	-0.731664	4.949355	-2.550619
H	-0.209280	5.579075	-3.273237
H	-1.273897	5.600751	-1.857782
C	-1.839225	2.888321	-2.113929
H	-2.666433	3.121852	-1.437512
H	-1.956161	1.874078	-2.490836
C	0.219018	4.035271	-1.801684
H	0.991909	3.633803	-2.462050
H	0.696863	4.487496	-0.931789
C	-1.678621	3.940387	-3.200642
H	-2.637586	4.372040	-3.492592
H	-1.217274	3.504175	-4.091141
F	-2.196627	-2.635118	0.085779
F	-1.937162	1.730959	1.270633
F	-3.859146	-1.232008	-1.867516
F	0.096018	0.194089	-2.922007
F	-4.402240	2.304223	2.230860
F	-6.614484	1.065041	1.166724
F	-1.372401	-4.774683	-1.310457
F	-6.269835	-0.699453	-0.881987
F	0.970421	-1.961612	-4.272531
F	0.231217	-4.471301	-3.492110
O	0.606723	2.936776	1.332436
N	-1.471584	0.008685	-0.672142
C	-3.028456	1.092791	0.750874
C	-1.100881	-1.133542	-1.377010
C	-2.772493	0.169357	-0.273737
C	-5.392363	0.788006	0.709250
C	-3.940734	-0.402717	-0.817437
C	-4.274920	1.410512	1.248139
C	-1.438074	-2.441559	-1.000232
C	-0.192786	-3.405234	-2.817065
C	-1.013430	-3.555262	-1.707147
C	-0.268998	-1.030608	-2.497317
C	-5.207701	-0.117148	-0.327883
C	0.186005	-2.129447	-3.207402
C	0.731408	4.949336	2.550804
H	0.208996	5.579031	3.273424
H	1.273637	5.600757	1.857987
C	1.839031	2.888340	2.114099
H	2.666241	3.121911	1.437698
H	1.955995	1.874095	2.490989
C	-0.219238	4.035239	1.801839
H	-0.992133	3.633746	2.462185
H	-0.697077	4.487466	0.931941
C	1.678379	3.940382	3.200829
H	2.637327	4.372055	3.492804
H	1.217026	3.504141	4.091310

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MgN^{F}_{2}·$(THF)_2$-F(-)

Mg	0.000000	0.000000	0.693763
O	-0.525590	2.167255	0.770326
O	0.525590	-2.167255	0.770326
C	-1.143806	4.179653	1.835486
C	1.143806	-4.179653	1.835486
H	-1.073182	4.715926	2.784913
H	1.073182	-4.715926	2.784913
H	-2.092976	4.448801	1.360035
H	2.092976	-4.448801	1.360035
C	0.000000	3.246428	-0.023028
C	0.000000	-3.246428	-0.023028
H	-0.665146	3.400439	-0.879509
H	0.665146	-3.400439	-0.879509
H	0.985910	2.950094	-0.384663
H	-0.985910	-2.950094	-0.384663
C	-1.044095	2.672913	2.022599
C	1.044095	-2.672913	2.022599
H	-0.354353	2.380789	2.816167
H	0.354353	-2.380789	2.816167
H	-2.004128	2.189184	2.207989
H	2.004128	-2.189184	2.207989
C	0.026422	4.463692	0.892396
C	-0.026422	-4.463692	0.892396
H	-0.080465	5.398286	0.335966
H	0.080465	-5.398286	0.335966
H	0.965494	4.500036	1.450541
H	-0.965494	-4.500036	1.450541
F	-4.257021	-1.966885	-0.916477
F	4.257021	1.966885	-0.916477
F	-2.129358	-2.232707	2.132655
F	2.129358	2.232707	2.132655
F	-4.089338	1.495587	-0.034976
F	4.089338	-1.495587	-0.034976
F	-0.801052	1.092786	-1.985086
F	0.801052	-1.092786	-1.985086
F	-3.855714	-1.953211	4.150029
F	3.855714	1.953211	4.150029
F	-5.764391	-0.004795	4.090055
F	5.764391	0.004795	4.090055
F	-5.047884	-1.941762	-3.467688
F	5.047884	1.941762	-3.467688
F	-5.871322	1.693472	1.953033
F	5.871322	-1.693472	1.953033
F	-1.573374	1.050596	-4.550023
F	1.573374	-1.050596	-4.550023
F	-3.717468	-0.457309	-5.336214
F	3.717468	0.457309	-5.336214
N	-2.025383	-0.434223	-0.024257
N	2.025383	0.434223	-0.024257
C	-2.992842	-1.215672	2.080471

C	2.992842	1.215672	2.080471
C	-2.484107	-0.429327	-1.319487
C	2.484107	0.429327	-1.319487
C	-2.994456	-0.360914	0.966394
C	2.994456	0.360914	0.966394
C	-4.881099	-0.119373	3.089371
C	4.881099	0.119373	3.089371
C	-4.010394	0.613512	0.974841
C	4.010394	-0.613512	0.974841
C	-3.898260	-1.096582	3.122422
C	3.898260	1.096582	3.122422
C	-3.583773	-1.185109	-1.779124
C	3.583773	1.185109	-1.779124
C	-3.323788	-0.447655	-4.055072
C	3.323788	0.447655	-4.055072
C	-4.001038	-1.190515	-3.099946
C	4.001038	1.190515	-3.099946
C	-1.836880	0.306700	-2.327498
C	1.836880	-0.306700	-2.327498
C	-4.936936	0.733497	1.998228
C	4.936936	-0.733497	1.998228
C	-2.228274	0.302782	-3.654453
C	2.228274	-0.302782	-3.654453
F	0.000000	0.000000	2.554177

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$(MgNF_2)_2$

Mg	-1.548244	0.165096	-0.078844
F	-1.310114	1.965522	-1.327014
F	-1.744788	-1.982614	0.398831
F	-3.956782	1.380784	-2.485006
F	1.766877	-0.547507	-3.859670
F	-6.310187	-1.154594	-0.535070
F	2.043236	-2.206171	-1.112552
F	-2.098757	-1.245903	-3.109499
F	-1.159296	3.974650	-3.141602
F	1.876814	-4.773550	-1.988771
F	1.872141	1.414353	-5.673231
F	0.438125	3.697608	-5.346724
F	-2.297744	-4.616618	0.712166
F	-6.800045	2.657048	1.962210
F	-2.243818	-3.777547	-4.035621
F	-5.119101	0.544907	2.009949
F	-0.275275	-5.559219	-3.468644
F	-5.605898	3.508605	-2.510796
F	-7.045120	4.156218	-0.293808
F	-6.837149	-3.732822	-0.190812
F	-4.883388	-5.525889	0.426704
N	-3.552372	-0.160043	-0.196356
N	0.063930	-0.349911	-1.523619
C	0.188024	0.633193	-2.544089
C	-0.515344	1.826161	-2.429101

C	-0.035811	-1.670460	-2.055181
C	-3.045470	-2.431555	0.258766
C	-3.995485	-1.448685	-0.046745
C	-4.483105	0.891361	-0.233921
C	0.954606	-2.613061	-1.806795
C	-4.637123	1.683904	-1.373212
C	-1.114860	-2.101270	-2.829448
C	-5.298034	-1.963767	-0.199216
C	0.353908	2.724218	-4.451897
C	-1.198458	-3.400674	-3.311284
C	1.082571	1.552861	-4.616940
C	-3.291907	-3.778103	0.420955
C	-5.486776	2.780979	-1.402506
C	-6.100881	2.340927	0.874923
C	-0.457337	2.868061	-3.333500
C	1.010527	0.536077	-3.672258
C	-5.236468	1.258139	0.885862
C	-6.225540	3.110154	-0.275154
C	0.900254	-3.918980	-2.259855
C	-0.192701	-4.315507	-3.021025
C	-5.586240	-3.311933	-0.032953
C	-4.594091	-4.234551	0.277921
Mg	1.548242	-0.165439	0.077948
F	1.310001	-1.965785	1.325714
F	1.744531	1.982145	-0.400346
F	3.955071	-1.381351	2.485533
F	-1.766928	0.546980	3.858716
F	6.309352	1.155783	0.537894
F	-2.042379	2.206710	1.111355
F	2.098611	1.244617	3.109535
F	1.158919	-3.975284	3.139904
F	-1.875190	4.773916	1.987791
F	-1.872456	-1.415258	5.671888
F	-0.438617	-3.698552	5.344988
F	2.296949	4.616238	-0.713871
F	6.802200	-2.655134	-1.959921
F	2.244397	3.776095	4.035856
F	5.120747	-0.543418	-2.008178
F	0.276772	5.558624	3.468383
F	5.604706	-3.508732	2.511801
F	7.045875	-4.155119	0.295719
F	6.835845	3.734095	0.193329
F	4.882063	5.526378	-0.426371
N	3.552150	0.160348	0.197191
N	-0.063886	0.349647	1.522683
C	-0.188153	-0.633630	2.542967
C	0.515140	-1.826618	2.427777
C	0.036216	1.670080	2.054458
C	3.044926	2.431544	-0.259112
C	3.994991	1.449070	0.047516
C	4.483099	-0.890849	0.235078
C	-0.953768	2.613091	1.805875

C	4.636401	-1.683814	1.374175
C	1.115179	2.100386	2.829138
C	5.297261	1.964573	0.200932
C	-0.354276	-2.724994	4.450353
C	1.199128	3.399716	3.311124
C	-1.082855	-1.553608	4.615600
C	3.291103	3.778116	-0.421506
C	5.486300	-2.780696	1.403702
C	6.102105	-2.339610	-0.873060
C	0.457020	-2.868685	3.331975
C	-1.010686	-0.536640	3.671127
C	5.237432	-1.257034	-0.884255
C	6.226047	-3.109253	0.276816
C	-0.899033	3.918945	2.259085
C	0.193840	4.314981	3.020623
C	5.585202	3.312772	0.034512
C	4.593029	4.234995	-0.277478

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MgN^{F}_{2}

Mg	-0.000299	-0.002985	0.003008
F	-0.595654	1.597086	1.504106
F	0.590346	1.493103	-1.600979
F	0.615508	-1.509353	1.606354
F	-4.627311	1.006108	-0.859256
F	4.627140	-0.865028	-1.011476
F	-0.609937	-1.609141	-1.494017
F	-4.635036	-0.994268	0.879177
F	-1.526340	3.970097	2.484361
F	-1.558684	-3.974680	-2.473475
F	-5.555670	3.309648	0.139774
F	-4.044377	4.822828	1.818546
F	1.517676	2.471293	-3.975319
F	5.583245	-0.125246	3.280645
F	-5.579008	-3.289912	-0.120639
F	4.631694	0.873611	0.985046
F	-4.081602	-4.812134	-1.803040
F	1.569846	-2.487319	3.971363
F	4.091561	-1.811267	4.803270
F	5.551408	0.134189	-3.316931
F	4.037188	1.808019	-4.830176
N	2.012077	-0.003616	-0.001404
N	-2.012428	-0.002353	0.007420
C	-2.639949	1.148831	0.427202
C	-1.881664	2.004670	1.236059
C	-2.648266	-1.149451	-0.407708
C	1.877837	1.223855	-2.010168
C	2.636238	0.416123	-1.153572
C	2.650342	-0.419888	1.144564
C	-1.898704	-2.010245	-1.219569
C	1.901159	-1.233700	2.004848
C	-3.898817	-1.652749	-0.020103

C	3.884243	0.030989	-1.666386
C	-3.583531	3.661400	1.363446
C	-4.379541	-2.863466	-0.501807
C	-4.358549	2.875489	0.519100
C	2.303872	1.700341	-3.232039
C	2.343608	-1.709583	3.221130
C	4.384156	-0.508339	2.855184
C	-2.310385	3.226000	1.711723
C	-3.886553	1.660916	0.038737
C	3.900165	-0.028070	1.645373
C	3.619044	-1.357036	3.645989
C	-2.336117	-3.227001	-1.698178
C	-3.612170	-3.653678	-1.348870
C	4.354127	0.511576	-2.881397
C	3.577467	1.354498	-3.667593

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(MgN^{F}_{2})-F(-)

Mg	0.165025	-0.194858	-1.558257
N	1.728447	0.349175	-0.276177
F	-1.360095	2.097783	-0.818779
N	-1.627839	-0.581291	-0.542544
F	2.116141	-1.241151	-2.368814
F	0.408597	-0.091234	2.136479
F	-4.244887	-1.633764	-1.106113
F	4.124087	0.944916	1.323968
F	0.157465	-2.516139	-0.872755
F	-3.554188	-0.971335	1.611737
F	-3.378308	3.708301	-1.605537
F	0.247352	-4.749411	0.666410
F	-6.255587	-0.014899	-1.828588
F	-5.856050	2.669219	-2.101889
F	4.520308	-2.275678	-3.045482
F	1.972134	4.985816	1.006046
F	-3.490711	-3.202527	3.082819
F	2.580220	2.990696	-0.704758
F	-1.599919	-5.120472	2.657730
F	-0.229662	1.913614	3.814830
F	0.552133	4.463604	3.269097
F	6.479527	-0.054946	0.617416
F	6.749229	-1.681262	-1.559873
C	-2.729017	0.178253	-0.875446
C	-2.569347	1.560919	-1.056946
C	-1.729833	-1.682523	0.260476
C	3.206532	-0.934483	-1.622027
C	3.000062	-0.076654	-0.523461
C	1.502526	1.377921	0.642171
C	-0.766591	-2.693329	0.108973
C	0.780573	1.151586	1.818353
C	-2.636623	-1.903419	1.313680
C	4.172783	0.181405	0.216806
C	-4.851703	1.872401	-1.716505

C	-2.600244	-3.046087	2.097253
C	-5.052541	0.508821	-1.565403
C	4.422827	-1.474866	-1.981372
C	0.454243	2.174641	2.696898
C	1.583492	3.735178	1.273031
C	-3.591206	2.396832	-1.466940
C	-4.010213	-0.314290	-1.170421
C	1.889365	2.702234	0.402024
C	0.857348	3.473093	2.425991
C	-0.697707	-3.830954	0.885713
C	-1.634208	-4.021187	1.893154
C	5.408713	-0.344156	-0.131139
C	5.552457	-1.175327	-1.230804
F	-0.210528	0.341873	-3.255523

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$MgN^{F}_{2}\cdot(Et_2O)_2$

Mg	0.000000	0.000000	1.379586
F	1.996617	-1.200098	1.678382
F	-1.996617	1.200098	1.678382
O	1.003381	1.110990	2.990155
O	-1.003381	-1.110990	2.990155
C	1.526321	2.446978	2.748106
C	-1.526321	-2.446978	2.748106
C	0.702346	3.531678	3.411208
C	-0.702346	-3.531678	3.411208
H	1.525172	2.571516	1.666876
H	-1.525172	-2.571516	1.666876
C	1.715369	0.389830	4.023237
C	-1.715369	-0.389830	4.023237
H	2.754745	0.271654	3.698941
H	-2.754745	-0.271654	3.698941
H	1.257671	-0.598902	4.040404
H	-1.257671	0.598902	4.040404
F	-1.069432	2.017171	-2.609047
F	1.069432	-2.017171	-2.609047
F	0.123940	4.291345	-1.191229
F	-0.123940	-4.291345	-1.191229
F	2.688848	1.021043	0.075626
F	-2.688848	-1.021043	0.075626
F	-3.905728	3.037449	2.241331
F	3.905728	-3.037449	2.241331
F	-3.823080	5.511235	1.046048
F	3.823080	-5.511235	1.046048
F	0.463018	1.850991	-4.800773
F	-0.463018	-1.850991	-4.800773
F	-1.780208	6.074419	-0.666815
F	1.780208	-6.074419	-0.666815
F	4.195902	0.787435	-2.134795
F	-4.195902	-0.787435	-2.134795
F	3.107285	1.219734	-4.602039
F	-3.107285	-1.219734	-4.602039

N	0.000000	1.607869	-0.001724
N	0.000000	-1.607869	-0.001724
C	-1.964516	2.417400	1.060225
C	1.964516	-2.417400	1.060225
C	0.754092	1.554485	-1.171643
C	-0.754092	-1.554485	-1.171643
C	-0.907583	2.625157	0.163511
C	0.907583	-2.625157	0.163511
C	-2.896529	4.592179	0.772603
C	2.896529	-4.592179	0.772603
C	-0.881956	3.921996	-0.386708
C	0.881956	-3.921996	-0.386708
C	-2.939563	3.341553	1.373403
C	2.939563	-3.341553	1.373403
C	0.233000	1.742422	-2.460765
C	-0.233000	-1.742422	-2.460765
C	2.357093	1.324358	-3.507602
C	-2.357093	-1.324358	-3.507602
C	1.011152	1.650425	-3.603810
C	-1.011152	-1.650425	-3.603810
C	2.112357	1.220471	-1.124708
C	-2.112357	-1.220471	-1.124708
C	-1.857214	4.868779	-0.106500
C	1.857214	-4.868779	-0.106500
C	2.905645	1.100580	-2.253738
C	-2.905645	-1.100580	-2.253738
C	1.654215	1.025130	5.397960
C	-1.654215	-1.025130	5.397960
H	2.567319	2.464742	3.085358
H	-2.567319	-2.464742	3.085358
H	2.138889	0.350818	6.110569
H	-2.138889	-0.350818	6.110569
H	2.186481	1.977434	5.442342
H	-2.186481	-1.977434	5.442342
H	0.625297	1.183752	5.729214
H	-0.625297	-1.183752	5.729214
H	1.119556	4.506671	3.141136
H	-1.119556	-4.506671	3.141136
H	-0.331380	3.509176	3.059867
H	0.331380	-3.509176	3.059867
H	0.701362	3.455718	4.499729
H	-0.701362	-3.455718	4.499729

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$MgN^{F}{}_{2}\cdot(Et_2O)_2$-F(-)

Mg	0.000000	0.000000	-0.366563
F	-2.107244	1.945458	0.213590
F	2.107244	-1.945458	0.213590
O	1.273106	2.359943	4.813893
O	-1.273106	-2.359943	4.813893
C	2.204037	3.155743	5.508527
C	-2.204037	-3.155743	5.508527

C	1.446673	4.147527	6.367709
C	-1.446673	-4.147527	6.367709
H	2.852274	3.686851	4.790795
H	-2.852274	-3.686851	4.790795
C	1.852966	1.455640	3.878948
C	-1.852966	-1.455640	3.878948
H	2.576091	2.000700	3.251117
H	-2.576091	-2.000700	3.251117
H	1.039608	1.122917	3.231106
H	-1.039608	-1.122917	3.231106
F	0.248443	4.499397	-2.450947
F	-0.248443	-4.499397	-2.450947
F	2.089689	4.071886	-0.200710
F	-2.089689	-4.071886	-0.200710
F	1.710518	0.013247	-2.150052
F	-1.710518	-0.013247	-2.150052
F	-2.821336	3.736794	2.100696
F	2.821336	-3.736794	2.100696
F	-1.105401	5.734539	2.820177
F	1.105401	-5.734539	2.820177
F	1.577190	4.770503	-4.745858
F	-1.577190	-4.770503	-4.745858
F	1.347066	5.882536	1.640042
F	-1.347066	-5.882536	1.640042
F	3.014302	0.289805	-4.512257
F	-3.014302	-0.289805	-4.512257
F	2.973324	2.694036	-5.831388
F	-2.973324	-2.694036	-5.831388
N	0.337686	1.960631	-0.993411
N	-0.337686	-1.960631	-0.993411
C	-1.240872	2.912419	0.554646
C	1.240872	-2.912419	0.554646
C	0.978886	2.248186	-2.163899
C	-0.978886	-2.248186	-2.163899
C	0.000000	2.959899	-0.094884
C	0.000000	-2.959899	-0.094884
C	-0.750641	4.840965	1.891146
C	0.750641	-4.840965	1.891146
C	0.857341	3.987552	0.321984
C	-0.857341	-3.987552	0.321984
C	-1.618609	3.822318	1.526122
C	1.618609	-3.822318	1.526122
C	0.959906	3.451660	-2.896084
C	-0.959906	-3.451660	-2.896084
C	2.333807	2.545408	-4.664012
C	-2.333807	-2.545408	-4.664012
C	1.629916	3.599960	-4.101099
C	-1.629916	-3.599960	-4.101099
C	1.691882	1.210143	-2.790298
C	-1.691882	-1.210143	-2.790298
C	0.492028	4.918269	1.280774
C	-0.492028	-4.918269	1.280774

C	2.352028	1.328107	-3.995751
C	-2.352028	-1.328107	-3.995751
C	2.519589	0.251028	4.526320
C	-2.519589	-0.251028	4.526320
H	2.860649	2.537575	6.140759
H	-2.860649	-2.537575	6.140759
H	2.867395	-0.433804	3.747513
H	-2.867395	0.433804	3.747513
H	3.384143	0.526169	5.138860
H	-3.384143	-0.526169	5.138860
H	1.805343	-0.290291	5.152327
H	-1.805343	0.290291	5.152327
H	2.143223	4.788290	6.917650
H	-2.143223	-4.788290	6.917650
H	0.805843	4.780680	5.749124
H	-0.805843	-4.780680	5.749124
H	0.814452	3.623721	7.089738
H	-0.814452	-3.623721	7.089738
F	0.000000	0.000000	1.462794

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$MgN"_2$

N	-1.945215	0.000719	0.000674
Si	-2.664538	-1.249609	0.952217
Mg	-0.001140	0.000106	0.000447
Si	2.665387	-0.954046	-1.246708
Si	2.664207	0.954743	1.246467
N	1.942754	-0.000507	0.000220
Si	-2.666109	1.249198	-0.952136
C	-3.921386	2.294362	-0.007084
H	-4.799104	1.705201	0.277694
H	-4.276271	3.130182	-0.619832
H	-3.488653	2.707575	0.909036
C	-3.503955	0.604194	-2.515928
H	-2.804264	0.032342	-3.133729
H	-3.894699	1.426864	-3.124827
H	-4.343055	-0.055735	-2.275753
C	-3.504166	-0.607063	2.515994
H	-2.805919	-0.033847	3.134130
H	-3.893266	-1.430784	3.124517
H	-4.344655	0.051079	2.275743
C	-3.917473	-2.296574	0.006138
H	-4.796223	-1.708812	-0.278352
H	-4.270903	-3.133454	0.618270
H	-3.483792	-2.708341	-0.910169
C	-1.252493	2.397395	-1.499847
H	-0.760591	2.888946	-0.651591
H	-1.633606	3.198339	-2.142304
H	-0.482877	1.882589	-2.091253
C	-1.249014	-2.395735	1.499708
H	-0.756729	-2.886832	0.651406
H	-1.628730	-3.197132	2.142445

H	-0.479841	-1.879936	2.090801
C	3.931571	0.015316	2.282300
C	3.488774	2.525097	0.600075
C	1.253446	1.491572	2.403418
H	1.634494	2.136312	3.202627
H	0.476004	2.077746	1.894113
H	0.770970	0.638921	2.896755
H	3.878675	3.135558	1.421998
H	4.326833	2.291561	-0.063686
H	2.782645	3.138982	0.031847
H	4.289665	0.629342	3.115797
H	3.506635	-0.903296	2.698167
H	4.806327	-0.264530	1.686291
C	3.928323	-0.011620	-2.285097
C	3.495848	-2.520999	-0.599424
C	1.255020	-1.496607	-2.401299
H	4.287244	-0.625360	-3.118449
H	3.499828	0.905182	-2.701339
H	4.802953	0.271756	-1.690589
H	3.888327	-3.130469	-1.420849
H	4.332781	-2.283830	0.064450
H	2.791878	-3.137216	-0.031041
H	1.637364	-2.140045	-3.200900
H	0.480851	-2.085561	-1.890321
H	0.768390	-0.646078	-2.894208

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MgN''_2-F(-)

N	-1.828513	0.051166	0.019638
Si	-2.960763	-0.863866	-0.890374
Mg	-0.007931	0.166809	-0.893128
Si	2.983742	1.049078	-0.590543
Si	2.164244	-1.513055	0.854724
N	1.824937	-0.105198	-0.058640
Si	-2.189858	1.159904	1.274826
C	-0.811096	1.194096	2.572433
H	-0.777104	0.246453	3.120257
H	-0.968303	1.999228	3.299835
H	0.172962	1.336816	2.114086
C	-3.792504	0.787073	2.230295
H	-4.675921	0.805539	1.583456
H	-3.943290	1.538462	3.014658
H	-3.750443	-0.195048	2.711989
C	-3.907239	-2.156817	0.134987
H	-3.208692	-2.814497	0.663091
H	-4.533422	-2.782286	-0.513011
H	-4.559129	-1.694722	0.882350
C	-4.276226	0.189990	-1.769379
H	-4.876088	0.766773	-1.056706
H	-4.964061	-0.430400	-2.356559
H	-3.793599	0.899424	-2.449373
C	-2.377800	2.941587	0.636518

H	-1.467155	3.279752	0.129978
H	-2.588854	3.646463	1.450007
H	-3.193775	3.008590	-0.090948
C	-2.055402	-1.833925	-2.243812
H	-1.472855	-1.166879	-2.890243
H	-2.773601	-2.371215	-2.874179
H	-1.378441	-2.583985	-1.818006
C	3.656979	-2.505950	0.211587
C	2.527107	-1.182668	2.690952
C	0.688443	-2.701282	0.802780
H	0.839752	-3.543227	1.488330
H	-0.242247	-2.197849	1.085606
H	0.551027	-3.119209	-0.201094
H	2.702229	-2.118715	3.235290
H	3.414412	-0.553384	2.813686
H	1.688102	-0.665959	3.166743
H	3.805954	-3.417884	0.802540
H	3.506936	-2.800988	-0.832332
H	4.585203	-1.926415	0.260408
C	4.330202	1.428786	0.701780
C	3.888342	0.528955	-2.174458
C	2.128812	2.695155	-0.974498
H	5.016332	2.196374	0.323887
H	3.889869	1.800921	1.632784
H	4.929519	0.545380	0.946988
H	4.595829	1.296482	-2.511230
H	4.444551	-0.403244	-2.029891
H	3.156332	0.365052	-2.971711
H	2.852419	3.437864	-1.330715
H	1.378380	2.558621	-1.761996
H	1.637644	3.111522	-0.087629
F	0.017657	0.707094	-2.661751

4

F2CO

C	-0.144287	0.000000	-0.000104
F	0.632294	-1.062541	0.000021
F	0.632294	1.062541	0.000021
O	-1.314446	0.000000	0.000031

5

F3CO(-)

C	0.002417	0.013409	-0.194204
F	0.649456	1.060759	0.540585
F	-1.281298	-0.010606	0.445776
F	0.615474	-1.143723	0.391775
O	0.016601	0.095209	-1.404750

3

MgI2

Mg	0.000111	0.000628	-0.000748
I	0.405364	-0.222738	-2.505861

I -0.405389 0.222596 2.506031

4
MgI2-F(-)
Mg 0.000000 -1.010110 0.000000
I 2.305261 0.352355 0.000000
I -2.305267 0.352267 0.000000
F 0.000037 -2.802628 0.000000

3
CaI2
Ca -0.000017 -0.000569 -0.000030
I 0.431782 0.397594 2.769895
I -0.431775 -0.397380 -2.769883

4
CaI2-F(-)
Ca 0.000000 -0.982586 0.000000
I 2.622277 0.439135 0.000000
I -2.622277 0.439138 0.000000
F -0.000002 -2.988527 0.000000

3
SrI2
Sr 0.000000 0.481250 0.000000
I 2.921118 -0.172523 0.000000
I -2.921118 -0.172524 0.000000

4
SrI2-F(-)
Sr 0.000000 0.886425 0.000000
I -2.787638 -0.574309 0.000000
I 2.787638 -0.574326 0.000000
F 0.000001 3.021498 0.000000

3
BaI2
Ba 0.000000 0.000000 0.882661
I 0.000000 2.826050 -0.466312
I 0.000000 -2.826050 -0.466312

4
BaI2-F(-)
Ba 0.000000 0.800822 0.000000
I 2.979410 -0.682634 0.000000
I -2.979409 -0.682634 0.000000
F -0.000001 3.057019 0.000000

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$CaN^{F}{}_{2}\cdot(THF)_{2}$
Ca -0.000022 1.340782 0.000001
F -0.004649 -0.083040 2.490716

F	2.132465	1.786125	-1.328046
F	2.822498	-2.708195	-0.231310
F	6.841694	1.439718	-1.301590
F	4.293906	-1.220602	1.617983
F	4.534751	2.578659	-2.263873
F	-0.855644	-2.319046	3.750982
F	6.655727	-0.460382	0.644915
F	0.154214	-4.762223	3.048443
F	1.999257	-4.916553	1.052074
O	-0.697516	3.055691	-1.547764
N	1.820093	-0.110060	0.513958
C	1.496482	-1.300697	1.136090
C	3.093879	0.170703	0.105465
C	3.265670	1.178979	-0.858242
C	0.061168	-2.416742	2.789098
C	0.520586	-1.284164	2.142354
C	4.482391	1.616869	-1.339287
C	1.955366	-2.579376	0.780208
C	5.649240	1.046097	-0.850227
C	4.309055	-0.339205	0.608279
C	1.522236	-3.729455	1.421967
C	0.574017	-3.657146	2.434735
C	5.546076	0.069264	0.131935
C	-0.807554	4.869243	-3.067647
H	-0.256778	5.340425	-3.883689
H	-1.357781	5.649650	-2.532939
C	-1.759708	3.767567	-3.535470
H	-2.701637	4.150448	-3.932291
H	-1.288109	3.152113	-4.307125
C	-1.960171	2.963541	-2.263006
H	-2.742966	3.396263	-1.630667
H	-2.174228	1.906987	-2.425887
C	0.113499	4.114167	-2.121533
H	0.951619	3.654167	-2.652036
H	0.504535	4.724607	-1.304531
F	0.004653	-0.083027	-2.490725
F	-2.132517	1.786051	1.328051
F	-2.822407	-2.708268	0.231306
F	-6.841739	1.439546	1.301580
F	-4.293895	-1.220654	-1.618048
F	-4.534821	2.578516	2.263889
F	0.855727	-2.319009	-3.750981
F	-6.655729	-0.460509	-0.644963
F	-0.154050	-4.762217	-3.048435
F	-1.999089	-4.916603	-1.052068
O	0.697429	3.055686	1.547793
N	-1.820099	-0.110100	-0.513977
C	-1.496449	-1.300728	-1.136107
C	-3.093894	0.170630	-0.105487
C	-3.265709	1.178886	0.858237
C	-0.061088	-2.416731	-2.789102
C	-0.520549	-1.284166	-2.142366

C	-4.482439	1.616742	1.339288
C	-1.955284	-2.579423	-0.780216
C	-5.649275	1.045956	0.850215
C	-4.309059	-0.339292	-0.608315
C	-1.522113	-3.729490	-1.421969
C	-0.573896	-3.657152	-2.434737
C	-5.546090	0.069145	-0.131967
C	0.807410	4.869210	3.067715
H	0.256613	5.340363	3.883758
H	1.357631	5.649638	2.533032
C	1.759578	3.767541	3.535529
H	2.701494	4.150432	3.932372
H	1.287980	3.152062	4.307164
C	1.960076	2.963547	2.263051
H	2.742870	3.396300	1.630732
H	2.174153	1.906993	2.425912
C	-0.113614	4.114136	2.121570
H	-0.951736	3.654112	2.652050
H	-0.504646	4.724587	1.304574

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$CaN^{F}{}_{2}\cdot(Et_2O)_2$

Ca	-0.000078	-1.336326	0.000059
F	-2.185275	-1.767337	1.263750
F	-4.224197	1.269786	-1.737014
F	-2.798094	2.739652	0.145839
F	2.798316	2.739551	-0.145809
F	-0.095740	0.082721	2.472403
F	2.185045	-1.767418	-1.263919
F	-4.623645	-2.528075	2.132286
F	-6.621394	0.542133	-0.829800
F	0.095783	0.082774	-2.472514
F	4.224281	1.269504	1.736815
F	-6.886633	-1.356326	1.108989
F	1.919268	4.935888	1.119925
F	-1.002504	2.306903	3.714743
F	0.012853	4.760061	3.055964
F	4.623340	-2.528345	-2.132540
F	-1.918818	4.936015	-1.119701
F	1.002767	2.306967	-3.714663
F	6.621412	0.541663	0.829538
F	6.886443	-1.356790	-1.109288
O	-0.619709	-3.075789	-1.578427
F	-0.012379	4.760160	-3.055716
O	0.619525	-3.075739	1.578604
N	1.795579	0.129532	0.561073
N	-1.795592	0.129614	-0.561202
C	-1.441351	1.316502	-1.174887
C	1.441457	1.316416	1.174820
C	-4.278646	0.389870	-0.727758
C	0.460197	3.660698	2.451866
C	-3.084874	-0.135259	-0.190161

C	1.439280	3.744060	1.469845
C	-1.901016	2.599854	-0.837749
C	1.901244	2.599753	0.837784
C	3.296485	-1.143624	-0.765762
C	-5.677189	-0.977691	0.692067
C	-0.055153	2.415229	2.784291
C	-3.296650	-1.143446	0.765554
C	-0.433323	1.288946	-2.148388
C	0.433448	1.288885	2.148343
C	-5.533843	-0.002015	-0.286113
C	3.084825	-0.135431	0.189971
C	-4.532267	-1.565164	1.211972
C	-1.756404	-2.876471	-2.447267
H	-1.401614	-2.775045	-3.477282
H	-2.160681	-1.908046	-2.148592
C	4.278647	0.389586	0.727555
C	-1.438940	3.744169	-1.469712
C	4.532058	-1.565439	-1.212212
C	5.677041	-0.978063	-0.692327
C	5.533803	-0.002390	0.285872
C	-0.459850	3.660791	-2.451724
C	0.182956	-4.238067	-1.861128
H	-0.426707	-5.135947	-1.710734
H	0.954646	-4.234290	-1.088896
C	0.055394	2.415301	-2.784233
C	1.756178	-2.876339	2.447484
H	1.401322	-2.774676	3.477454
H	2.160553	-1.908007	2.148641
C	-2.808996	-3.960750	-2.329930
H	-3.676755	-3.676870	-2.931879
H	-3.143746	-4.079607	-1.296202
H	-2.461245	-4.928766	-2.699426
C	-0.183198	-4.237948	1.861418
H	0.426431	-5.135871	1.711144
H	-0.954868	-4.234227	1.089164
C	0.818015	-4.234953	-3.237986
H	0.084167	-4.352539	-4.038611
H	1.511972	-5.077473	-3.307624
H	1.384427	-3.317513	-3.409398
C	-0.818290	-4.234642	3.238259
H	-1.512272	-5.077134	3.307987
H	-1.384683	-3.317166	3.409543
H	-0.084463	-4.352144	4.038917
C	2.808695	-3.960721	2.330441
H	2.460854	-4.928631	2.700129
H	3.676441	-3.676772	2.932377
H	3.143495	-4.079826	1.296758

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$CaN^{F}_{2}\cdot(THF)_{2}$-F(-)

Ca	0.000370	-0.905961	-0.000495
F	-0.505323	1.441632	1.294566

F	-2.243718	-1.607504	-2.385508
F	-4.572392	1.686370	-1.132530
F	-6.350662	-3.578335	-1.209831
F	-4.646885	-0.040686	1.377973
F	-4.156394	-3.439996	-2.832171
F	-0.771186	4.027954	1.970528
F	-6.568380	-1.840337	0.885963
F	-2.949101	5.471073	1.138659
F	-4.830875	4.238755	-0.411744
O	0.818104	-1.402963	-2.351182
N	-2.298598	0.116055	-0.249574
C	-2.540985	1.415162	0.086358
C	-3.352846	-0.734688	-0.490594
C	-3.289596	-1.657854	-1.549823
C	-1.709885	3.448865	1.213905
C	-1.595449	2.118665	0.859691
C	-4.270988	-2.602969	-1.794074
C	-3.630109	2.213212	-0.330317
C	-5.392653	-2.669706	-0.980552
C	-4.502998	-0.850006	0.313326
C	-3.770038	3.545458	0.021717
C	-2.813489	4.181085	0.799513
C	-5.501667	-1.779627	0.077232
C	2.028027	-2.969651	-3.576717
H	1.985816	-3.798735	-4.287710
H	2.819809	-3.178527	-2.851199
C	2.247832	-1.611498	-4.252791
H	3.302281	-1.379656	-4.418071
H	1.744013	-1.587145	-5.224003
C	1.588249	-0.620122	-3.279920
H	2.321852	-0.055756	-2.702237
H	0.926947	0.085035	-3.794297
C	0.711091	-2.746368	-2.855749
H	-0.136299	-2.804894	-3.552501
H	0.521551	-3.383692	-1.991715
F	0.506788	1.443535	-1.293572
F	2.240347	-1.609199	2.383606
F	4.574333	1.683108	1.133198
F	6.346065	-3.584288	1.210424
F	4.648549	-0.043194	-1.376871
F	4.150634	-3.444329	2.830992
F	0.774761	4.030111	-1.967740
F	6.567587	-1.845407	-0.884244
F	2.954058	5.470767	-1.135200
F	4.834950	4.235770	0.414111
O	-0.820832	-1.406942	2.347821
N	2.299173	0.115324	0.249151
C	2.542667	1.414433	-0.085835
C	3.352340	-0.736655	0.490337
C	3.287066	-1.660373	1.548968
C	1.713104	3.449671	-1.211720
C	1.597576	2.119302	-0.858463

C	4.267074	-2.606805	1.793512
C	3.632510	2.211279	0.331325
C	5.389342	-2.674375	0.980858
C	4.502941	-0.852887	-0.312759
C	3.773502	3.543658	-0.019744
C	2.817387	4.180650	-0.796968
C	5.500292	-1.783861	-0.076352
C	-2.030810	-2.973727	3.573154
H	-1.988574	-3.803781	4.283009
H	-2.823945	-3.180667	2.848553
C	-2.247900	-1.616175	4.251295
H	-3.301776	-1.383354	4.418848
H	-1.742214	-1.593600	5.221581
C	-1.589029	-0.624366	3.278414
H	-2.323070	-0.058964	2.702299
H	-0.926470	0.079848	3.792450
C	-0.714648	-2.751090	2.850576
H	0.133647	-2.811460	3.546066
H	-0.526747	-3.387537	1.985548
F	0.000856	-2.994701	-0.002129

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$CaN^{F}_{2}\cdot(Et_2O)_2$-F(-)

Ca	0.069140	-1.597219	-0.163967
F	2.456702	-1.440665	-1.202610
F	3.770946	1.892815	1.913100
F	1.519971	2.841455	0.194603
F	-3.188762	2.621598	-0.594900
F	0.461750	0.136953	-2.316353
F	-2.065665	-0.553829	1.987221
F	4.888880	-1.324254	-2.326676
F	6.151264	2.014174	0.749644
F	0.679586	-0.576945	3.349324
F	-3.969457	0.213157	-2.274325
F	6.784447	0.426751	-1.384640
F	-2.539976	4.653091	-2.190985
F	1.127700	2.223675	-3.880231
F	-0.377286	4.516698	-3.854670
F	-4.468416	-1.329625	2.912141
F	0.289914	4.613925	1.800597
F	-0.569679	1.200975	4.931295
F	-6.373386	-0.502346	-1.318242
F	-6.655834	-1.299916	1.278808
O	1.359130	-3.322547	1.221821
F	-0.780130	3.814651	4.178138
O	-0.097396	-2.909788	-2.405434
N	-1.636737	0.153716	-0.630592
N	1.697058	0.091743	0.869979
C	1.146931	1.054750	1.701291
C	-1.416048	1.249052	-1.412215
C	3.975248	1.119625	0.830588
C	-0.703988	3.475422	-3.074400

C	2.943190	0.267842	0.363150
C	-1.804915	3.534241	-2.233080
C	1.014113	2.410196	1.358255
C	-2.140147	2.462247	-1.421600
C	-3.109564	-0.546920	1.147172
C	5.565780	0.368203	-0.825597
C	0.057917	2.315599	-3.080964
C	3.355646	-0.546950	-0.714301
C	0.581125	0.693740	2.932090
C	-0.300917	1.255333	-2.273678
C	5.231894	1.178169	0.249730
C	-2.910656	-0.122253	-0.175986
C	4.604152	-0.512366	-1.300142
C	2.565363	-3.085704	1.953804
H	2.398589	-3.311490	3.013138
H	2.745026	-2.012453	1.880726
C	-4.064683	-0.131038	-0.976813
C	0.383391	3.333178	2.174810
C	-4.340385	-0.942964	1.637476
C	-5.456030	-0.923393	0.812840
C	-5.309007	-0.510643	-0.502089
C	-0.164385	2.930304	3.384447
C	0.650493	-4.511141	1.616093
H	1.365824	-5.341195	1.690503
H	-0.045878	-4.707104	0.801285
C	-0.062139	1.599889	3.759843
C	-1.355941	-2.597629	-3.024017
H	-1.209149	-2.606258	-4.114171
H	-1.571456	-1.570475	-2.725495
C	3.748004	-3.874235	1.415772
H	4.644423	-3.631882	1.995633
H	3.943787	-3.622198	0.370984
H	3.589724	-4.954347	1.486479
C	0.392427	-4.194755	-2.770696
H	0.279171	-4.313151	-3.859047
H	-0.211428	-4.972740	-2.286703
C	-0.136343	-4.334768	2.900666
H	0.497701	-4.084760	3.756142
H	-0.655696	-5.270357	3.134316
H	-0.886375	-3.555431	2.760858
C	1.845592	-4.333644	-2.377485
H	2.207305	-5.325837	-2.665003
H	1.971672	-4.227945	-1.297887
H	2.462334	-3.581925	-2.873568
C	-2.495305	-3.509134	-2.604110
H	-2.385463	-4.523201	-3.000326
H	-3.434706	-3.104517	-2.993190
H	-2.546583	-3.545370	-1.511982
F	-1.453972	-2.928343	0.347064

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(MgN“$_2$)$_2$

Mg	1.473650	0.000024	-0.000008
Mg	-1.466396	-0.000008	0.000025
N	3.478950	0.000011	0.000058
N	-0.001021	-1.598674	-0.042620
N	-3.473178	-0.000013	0.000076
Si	4.395863	0.708193	-1.304104
Si	0.472124	-2.411907	-1.566189
Si	-0.498394	-2.808263	1.195956
Si	-4.367826	-0.451837	-1.424851
C	3.342501	1.903756	-2.335139
H	4.006590	2.568755	-2.901871
H	2.700397	2.539023	-1.716868
H	2.715644	1.391117	-3.072996
C	5.876738	1.749767	-0.726583
H	6.384151	2.177839	-1.600912
H	6.624426	1.176945	-0.167604
H	5.554789	2.583588	-0.091132
C	5.055691	-0.561294	-2.552616
H	5.559916	-0.050184	-3.383426
H	4.240703	-1.158126	-2.979791
H	5.773838	-1.258288	-2.108662
C	0.755419	-1.104909	-2.906930
H	1.230252	-1.607647	-3.759223
H	1.443798	-0.296339	-2.627815
H	-0.161939	-0.642948	-3.279043
C	2.139637	-3.297608	-1.457547
H	2.429310	-3.616353	-2.467621
H	2.141387	-4.185433	-0.821511
H	2.918884	-2.616630	-1.095271
C	-0.810506	-3.617452	-2.257968
H	-0.497320	-3.918025	-3.266134
H	-1.808116	-3.173582	-2.341365
H	-0.900390	-4.531733	-1.662535
C	0.462279	-4.443755	1.204633
H	0.036341	-5.039877	2.022778
H	1.531394	-4.334312	1.408315
H	0.345842	-5.032447	0.289589
C	-2.307177	-3.307511	0.964237
H	-2.625387	-3.907716	1.826737
H	-2.453384	-3.920931	0.069221
H	-2.981090	-2.447571	0.884580
C	-0.368374	-2.173250	2.969139
H	-0.729640	-2.981048	3.619122
H	-0.994193	-1.302634	3.178801
H	0.654450	-1.944474	3.276892
C	-3.259141	-0.357046	-2.963215
H	-3.769963	-0.815991	-3.819056
H	-2.307637	-0.892023	-2.849989
H	-3.041841	0.681205	-3.236970
C	-5.063731	-2.217481	-1.398306
H	-5.632385	-2.409736	-2.317593
H	-5.738368	-2.386277	-0.552282

H	-4.270163	-2.970474	-1.337209
C	-5.830262	0.698359	-1.806076
H	-6.296258	0.402222	-2.754883
H	-5.506014	1.740839	-1.907377
H	-6.612117	0.666854	-1.038772
N	-0.001043	1.598697	0.042532
Si	4.395738	-0.708208	1.304288
Si	0.472083	2.412058	1.566037
Si	-0.498461	2.808165	-1.196136
Si	-4.367808	0.451805	1.425017
C	3.342246	-1.903726	2.335247
H	4.006268	-2.568774	2.902001
H	2.700143	-2.538946	1.716927
H	2.715374	-1.391070	3.073080
C	5.876604	-1.749852	0.726870
H	6.383939	-2.177947	1.601234
H	6.624356	-1.177064	0.167942
H	5.554660	-2.583659	0.091397
C	5.055531	0.561252	2.552846
H	5.559672	0.050123	3.383695
H	4.240535	1.158117	2.979959
H	5.773740	1.258216	2.108946
C	0.755453	1.105178	2.906873
H	1.230278	1.608002	3.759119
H	1.443864	0.296618	2.627808
H	-0.161877	0.643205	3.279035
C	2.139563	3.297807	1.457305
H	2.429238	3.616643	2.467350
H	2.141279	4.185579	0.821196
H	2.918826	2.616821	1.095074
C	-0.810587	3.617607	2.257730
H	-0.497416	3.918269	3.265875
H	-1.808180	3.173706	2.341155
H	-0.900504	4.531841	1.662229
C	0.462148	4.443694	-1.204970
H	0.036179	5.039716	-2.023172
H	1.531267	4.334284	-1.408641
H	0.345682	5.032469	-0.289982
C	-2.307261	3.307368	-0.964438
H	-2.625504	3.907490	-1.826982
H	-2.453477	3.920858	-0.069469
H	-2.981146	2.447413	-0.884701
C	-0.368445	2.172985	-2.969262
H	-0.729727	2.980711	-3.619325
H	-0.994243	1.302333	-3.178837
H	0.654382	1.944197	-3.276998
C	-3.259111	0.357017	2.963373
H	-3.769909	0.815994	3.819211
H	-2.307596	0.891969	2.850120
H	-3.041831	-0.681234	3.237147
C	-5.063717	2.217447	1.398477
H	-5.632352	2.409720	2.317771

H	-5.738369	2.386231	0.552462
H	-4.270148	2.970437	1.337351
C	-5.830239	-0.698396	1.806248
H	-6.296229	-0.402257	2.755057
H	-5.505988	-1.740875	1.907551
H	-6.612100	-0.666894	1.038950

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$(CaN^{F}2)2$

Ca	1.599817	-0.528774	-0.747647
F	0.391688	-1.222511	-2.787726
F	2.230545	1.505066	0.713123
F	3.098942	-1.926446	-2.343295
F	-2.550235	2.433141	-2.321814
F	6.472858	1.054724	-1.312308
F	-1.072718	2.947458	0.496796
F	1.496056	1.937935	-3.321803
F	-1.012845	-2.073058	-4.931758
F	-0.186171	5.501947	0.414708
F	-3.903796	1.615957	-4.497055
F	-3.169251	-0.647730	-5.812702
F	2.890966	4.007385	1.520289
F	7.797105	-2.859377	0.203510
F	2.336998	4.501307	-3.430911
F	6.365806	-0.678862	0.823281
F	1.517069	6.297273	-1.562742
F	4.534987	-4.154596	-2.935034
F	6.916562	-4.625130	-1.668711
F	7.122332	3.511063	-0.490726
F	5.369728	5.033086	0.932801
N	3.889770	-0.103109	-0.575697
N	-0.287667	1.029362	-1.341253
C	-1.015219	0.645329	-2.492601
C	-0.690274	-0.507230	-3.202870
C	0.165811	2.367736	-1.422181
C	3.487345	1.993965	0.453037
C	4.362609	1.136451	-0.226989
C	4.730921	-1.169662	-0.820371
C	-0.208996	3.326107	-0.484872
C	4.305404	-2.138606	-1.737611
C	1.048258	2.814843	-2.412816
C	5.597311	1.726423	-0.557181
C	-2.481614	-0.237483	-4.755905
C	1.497038	4.126279	-2.474570
C	-2.850629	0.922353	-4.084765
C	3.788881	3.279327	0.854612
C	5.005566	-3.290159	-2.040422
C	6.663177	-2.618404	-0.448277
C	-1.388465	-0.966218	-4.305209
C	-2.134082	1.339595	-2.972290
C	5.927540	-1.480158	-0.154004

C	6.212224	-3.529523	-1.395868
C	0.222212	4.640189	-0.505117
C	1.084124	5.045670	-1.516986
C	5.935434	3.011960	-0.159572
C	5.040619	3.799542	0.555511
Ca	-1.599720	0.528786	0.747830
F	-0.392054	1.222296	2.788245
F	-2.230529	-1.505450	-0.712985
F	-3.098974	1.926294	2.343379
F	2.550406	-2.432893	2.322049
F	-6.473023	-1.054505	1.311908
F	1.073030	-2.947221	-0.496581
F	-1.496091	-1.938143	3.321895
F	1.012302	2.072821	4.932399
F	0.186552	-5.501766	-0.414807
F	3.903780	-1.615748	4.497428
F	3.168867	0.647713	5.813272
F	-2.891170	-4.007675	-1.520196
F	-7.796688	2.859581	-0.204120
F	-2.336941	-4.501542	3.430710
F	-6.365437	0.679002	-0.823741
F	-1.516819	-6.297321	1.562437
F	-4.534954	4.154497	2.934950
F	-6.916325	4.625226	1.668284
F	-7.122734	-3.510739	0.490260
F	-5.370163	-5.033026	-0.933037
N	-3.889685	0.102995	0.575566
N	0.287754	-1.029328	1.341507
C	1.015156	-0.645303	2.492952
C	0.690014	0.507136	3.203325
C	-0.165688	-2.367717	1.422330
C	-3.487429	-1.994143	-0.453097
C	-4.362660	-1.136502	0.226809
C	-4.730767	1.169622	0.820179
C	0.209233	-3.326010	0.484979
C	-4.305343	2.138531	1.737496
C	-1.048183	-2.814946	2.412862
C	-5.597478	-1.726306	0.556863
C	2.481335	0.237475	4.756404
C	-1.496922	-4.126408	2.474462
C	2.850535	-0.922245	4.085166
C	-3.789087	-3.279478	-0.854670
C	-5.005466	3.290127	2.040240
C	-6.662874	2.618517	0.447832
C	1.388101	0.966103	4.305740
C	2.134087	-1.339469	2.972620
C	-5.927270	1.480234	0.153640
C	-6.212009	3.529588	1.395515
C	-0.221930	-4.640103	0.505062
C	-1.083910	-5.045701	1.516831
C	-5.935725	-3.011807	0.159237
C	-5.040933	-3.799522	-0.555722

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$CaN^{F}2$

Ca	0.000036	-0.000278	-0.000229
N	-2.325633	-0.000047	0.000062
F	0.979173	-0.840178	2.117070
N	2.325705	-0.000207	-0.000191
F	-0.979389	-2.117445	-0.840044
F	-0.978810	2.117197	0.839639
F	4.921075	-1.264600	-0.453466
F	-4.921212	0.453346	-1.263832
F	0.979181	0.839672	-2.117494
F	4.920890	1.264521	0.453275
F	1.980996	-2.606351	3.918542
F	1.980880	2.606023	-3.918853
F	5.912292	-2.970409	1.354358
F	4.481974	-3.670670	3.558540
F	-1.981576	-3.918810	-2.606119
F	-5.911744	1.355093	2.970545
F	5.911986	2.970507	-1.354440
F	-4.920952	-0.452892	1.264632
F	4.481703	3.670652	-3.558683
F	-1.980215	3.918843	2.605883
F	-4.481084	3.559135	3.670553
F	-5.912763	-1.354363	-2.969577
F	-4.482675	-3.558615	-3.670099
C	2.969765	-0.878210	0.837572
C	2.258174	-1.329585	1.959011
C	2.969699	0.877912	-0.837882
C	-2.258428	-1.959257	-1.329321
C	-2.969861	-0.837749	-0.877864
C	-2.969485	0.837846	0.878089
C	2.258114	1.329234	-1.959348
C	-2.257735	1.959256	1.329278
C	4.214271	1.505443	-0.655347
C	-4.214617	-0.655232	-1.505030
C	3.989853	-2.791593	2.689339
C	4.721853	2.418563	-1.568622
C	4.722077	-2.418610	1.568455
C	-2.725801	-2.876742	-2.247862
C	-2.724707	2.876877	2.247889
C	-4.721551	1.569010	2.418628
C	2.725355	-2.248183	2.876538
C	4.214429	-1.505584	0.655125
C	-4.214106	0.655577	1.505590
C	-3.989153	2.689826	2.791477
C	2.725228	2.247920	-2.876821
C	3.989645	2.791487	-2.689535
C	-4.722460	-1.568523	-2.417989
C	-3.990359	-2.689444	-2.791103

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CaN^F2-F

Ca	0.181535	0.674228	-1.146519
N	2.214227	-0.175700	-0.102097
F	-1.509090	-0.910392	-2.596557
N	-2.159121	0.524410	-0.422713
F	0.231666	-1.915834	-0.517109
F	2.187471	2.527190	-0.123378
F	-4.225471	-0.608770	1.260883
F	4.095744	-0.879804	2.013524
F	-0.545568	2.167907	0.922582
F	-4.953189	1.347027	-0.587554
F	-2.722505	-3.233707	-3.256586
F	-1.404612	4.407729	2.172374
F	-5.448372	-2.888143	0.569941
F	-4.724639	-4.240006	-1.685878
F	-0.056532	-4.208034	0.884538
F	6.886067	0.091129	-1.328969
F	-5.789910	3.539181	0.688030
F	4.735965	-1.403541	-0.745328
F	-4.051935	5.109641	2.085179
F	4.349310	4.018839	-0.758582
F	6.727279	2.813270	-1.356106
F	3.822013	-3.173522	3.351006
F	1.755295	-4.876644	2.831512
C	-2.875392	-0.611218	-0.694826
C	-2.514937	-1.374952	-1.819151
C	-2.719784	1.603985	0.196410
C	1.146150	-2.229344	0.438600
C	2.206689	-1.324263	0.632337
C	3.381274	0.506580	-0.357730
C	-1.866600	2.483381	0.889443
C	3.348121	1.910018	-0.413770
C	-4.060459	2.037490	0.138842
C	3.090081	-1.699159	1.666784
C	-4.125184	-3.086531	-1.366219
C	-4.502041	3.187738	0.772922
C	-4.497410	-2.388022	-0.226761
C	0.973871	-3.400258	1.148611
C	4.443044	2.686871	-0.743837
C	5.731760	0.692532	-1.017733
C	-3.110936	-2.572592	-2.162845
C	-3.875069	-1.195620	0.105809
C	4.618896	-0.067423	-0.696842
C	5.653738	2.077232	-1.042746
C	-2.280040	3.640617	1.518195
C	-3.620856	3.998775	1.473734
C	2.946874	-2.876260	2.383764
C	1.891484	-3.741811	2.133029
F	0.605890	1.708468	-2.838196

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(CaN”2)2

Ca	1.730035	0.000155	-0.000480
Ca	-1.729935	-0.000273	-0.000928
N	3.997185	0.000219	0.000959
N	0.000130	-1.786128	-0.001286
N	-3.997012	-0.000063	0.001015
Si	4.783862	0.730689	-1.344020
Si	0.492854	-2.745604	-1.397067
Si	-0.492216	-2.749282	1.392178
Si	-4.783369	-0.726413	-1.346379
C	3.442256	1.182709	-2.616488
H	3.874668	1.758100	-3.441910
H	2.651016	1.816056	-2.194715
H	2.984925	0.294216	-3.066869
C	5.700951	2.337538	-0.946948
H	6.121635	2.780713	-1.856751
H	6.529019	2.166282	-0.252589
H	5.038673	3.078444	-0.488920
C	6.011298	-0.389987	-2.248985
H	6.361942	0.083848	-3.172844
H	5.560728	-1.351581	-2.513854
H	6.894599	-0.597116	-1.636372
C	0.488827	-1.698617	-2.971979
H	0.938879	-2.294514	-3.773843
H	1.074693	-0.775503	-2.918852
H	-0.517952	-1.428943	-3.300721
C	2.276475	-3.351351	-1.219369
H	2.580176	-3.883300	-2.128079
H	2.396187	-4.040187	-0.379555
H	2.995912	-2.535074	-1.075339
C	-0.583048	-4.247184	-1.796207
H	-0.191732	-4.721636	-2.703221
H	-1.622922	-3.972802	-1.994832
H	-0.580948	-5.005246	-1.009066
C	0.584200	-4.251687	1.786761
H	0.192882	-4.729210	2.692160
H	1.623944	-3.977599	1.986434
H	0.582451	-5.007192	0.997167
C	-2.275622	-3.355147	1.212785
H	-2.579172	-3.889755	2.119982
H	-2.395035	-4.041686	0.371045
H	-2.995257	-2.538661	1.071024
C	-0.488362	-1.706636	2.969887
H	-0.937915	-2.304816	3.770322
H	-1.074859	-0.783818	2.918955
H	0.518300	-1.437088	3.299077
C	-3.441288	-1.175300	-2.619496
H	-3.873616	-1.747851	-3.446931
H	-2.650784	-1.810581	-2.199225
H	-2.983030	-0.285801	-3.066942
C	-5.701129	-2.334154	-0.954553
H	-6.121003	-2.774732	-1.865988
H	-6.529844	-2.164634	-0.260542

H	-5.039428	-3.076424	-0.497898
C	-6.009840	0.397512	-2.248604
H	-6.359431	-0.072759	-3.174679
H	-5.558964	1.360113	-2.509259
H	-6.893849	0.602295	-1.636222
N	-0.000287	1.785979	-0.000242
Si	4.783844	-0.730037	1.346096
Si	0.491667	2.745639	1.395696
Si	-0.492685	2.748971	-1.393793
Si	-4.784128	0.726089	1.348130
C	3.442486	-1.182225	2.618685
H	3.875048	-1.757632	3.444021
H	2.651244	-1.815545	2.196909
H	2.985117	-0.293780	3.069094
C	5.701230	-2.336721	0.948987
H	6.122001	-2.779849	1.858771
H	6.529258	-2.165319	0.254615
H	5.039066	-3.077730	0.490956
C	6.011167	0.390944	2.250852
H	6.361880	-0.082715	3.174774
H	5.560459	1.352507	2.515601
H	6.894439	0.598114	1.638209
C	0.488177	1.698425	2.970445
H	0.937571	2.294613	3.772463
H	1.074941	0.775875	2.917292
H	-0.518388	1.427777	3.299018
C	2.274955	3.352461	1.218397
H	2.578016	3.884827	2.127078
H	2.394606	4.041130	0.378441
H	2.994854	2.536499	1.074922
C	-0.585261	4.246494	1.794768
H	-0.194525	4.721046	2.701979
H	-1.625039	3.971475	1.993004
H	-0.583349	5.004677	1.007741
C	0.582907	4.252098	-1.787870
H	0.191498	4.729520	-2.693284
H	1.622851	3.978640	-1.987366
H	0.580546	5.007482	-0.998165
C	-2.276517	3.353765	-1.214868
H	-2.580373	3.887681	-2.122368
H	-2.396307	4.040727	-0.373521
H	-2.995761	2.537028	-1.072529
C	-0.487477	1.706616	-2.971705
H	-0.937286	2.304548	-3.772181
H	-1.073066	0.783210	-2.921169
H	0.519570	1.438085	-3.300572
C	-3.443327	1.174822	2.622488
H	-3.876397	1.747242	3.449631
H	-2.652493	1.810059	2.202844
H	-2.985373	0.285241	3.070038
C	-5.701620	2.333834	0.955592
H	-6.122273	2.774383	1.866681

H	-6.529737	2.164357	0.260854
H	-5.039525	3.076131	0.499541
C	-6.011452	-0.398035	2.248976
H	-6.361720	0.071980	3.174926
H	-5.560841	-1.360741	2.509704
H	-6.895008	-0.602564	1.635855

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CaN”2

N	-2.251833	-0.000176	-0.000017
Si	-2.872464	1.113159	-1.131477
Ca	0.000012	0.000169	-0.001121
Si	2.872496	1.131989	1.113000
Si	2.872216	-1.131997	-1.112781
N	2.251860	0.000114	0.000041
Si	-2.872243	-1.113244	1.131876
C	-3.885852	-2.521649	0.385296
H	-4.807518	-2.141394	-0.067262
H	-4.172146	-3.259664	1.142694
H	-3.327476	-3.041874	-0.399430
C	-3.885965	-0.343659	2.527717
H	-3.328060	0.450116	3.034541
H	-4.171452	-1.088805	3.278406
H	-4.808098	0.101705	2.140193
C	-3.886334	0.343962	-2.527419
H	-3.328097	-0.448967	-3.035204
H	-4.172846	1.089489	-3.277339
H	-4.807881	-0.102466	-2.139727
C	-3.885819	2.521548	-0.384558
H	-4.807621	2.141340	0.067761
H	-4.171862	3.259874	-1.141747
H	-3.327421	3.041379	0.400411
C	-1.337597	-1.921605	1.953553
H	-0.705838	-2.483213	1.249069
H	-1.648986	-2.657909	2.701714
H	-0.705821	-1.208228	2.503784
C	-1.337854	1.921626	-1.953329
H	-0.705945	2.483258	-1.248989
H	-1.649480	2.657989	-2.701333
H	-0.706174	1.208427	-2.503936
C	3.886940	-0.386137	-2.520755
C	3.884546	-2.528606	-0.342785
C	1.337403	-1.952736	-1.922003
H	1.648879	-2.701064	-2.658101
H	0.704831	-2.502768	-1.209153
H	0.706406	-1.247950	-2.484104
H	4.171039	-3.278809	-1.088032
H	4.806051	-2.141496	0.104233
H	3.325419	-3.035908	0.449826
H	4.172604	-1.143676	-3.258870
H	3.329512	0.399298	-3.040923
H	4.809005	0.065349	-2.140193

C	3.886613	0.385576	2.521122
C	3.885845	2.527886	0.343015
C	1.338020	1.953613	1.921732
H	4.171842	1.142815	3.259713
H	3.328977	-0.400123	3.040667
H	4.808912	-0.065659	2.140827
H	4.172979	3.277795	1.088313
H	4.807014	2.140134	-0.104138
H	3.327023	3.035714	-0.449477
H	1.649542	2.701901	2.657850
H	0.705963	2.503743	1.208512
H	0.706526	1.249073	2.483547

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CaN”2-F

N	2.074149	-0.110448	0.046903
Si	3.162429	1.038409	-0.584243
Ca	-0.006774	0.117287	-1.035645
Si	-3.153931	-1.055062	-0.621211
Si	-2.430673	1.410233	1.085223
N	-2.120321	0.159129	-0.021206
Si	2.404669	-1.435217	1.065641
C	0.903757	-1.843903	2.153592
H	0.704910	-1.027900	2.856247
H	1.074267	-2.755939	2.737851
H	-0.012798	-1.993228	1.572250
C	3.857807	-1.193578	2.273331
H	4.804095	-1.033676	1.744935
H	3.981880	-2.077057	2.911123
H	3.690819	-0.329867	2.925290
C	3.988396	2.153917	0.717855
H	3.232640	2.644970	1.340197
H	4.594642	2.935383	0.243535
H	4.642808	1.581674	1.382956
C	4.576816	0.309410	-1.626359
H	5.210215	-0.354636	-1.027408
H	5.219809	1.093136	-2.044771
H	4.173680	-0.278137	-2.457697
C	2.809023	-3.024883	0.098680
H	1.988453	-3.297911	-0.574242
H	2.990992	-3.876314	0.765868
H	3.700873	-2.885152	-0.521811
C	2.214175	2.224194	-1.735528
H	1.708838	1.707698	-2.562408
H	2.908790	2.940432	-2.189015
H	1.474301	2.822496	-1.187166
C	-3.991783	2.437312	0.718365
C	-2.601562	0.845509	2.892478
C	-0.980033	2.644232	1.054164
H	-1.119391	3.434134	1.801060
H	-0.020965	2.161343	1.280244
H	-0.894448	3.141316	0.079844

H	-2.741181	1.694865	3.572264
H	-3.458265	0.174296	3.014714
H	-1.709403	0.297603	3.211935
H	-4.093240	3.276127	1.417723
H	-3.962200	2.844615	-0.297759
H	-4.898148	1.827199	0.801863
C	-4.148590	-1.982599	0.711394
C	-4.425766	-0.435516	-1.889993
C	-2.110467	-2.365613	-1.522627
H	-4.731427	-2.802135	0.273789
H	-3.484897	-2.407572	1.471640
H	-4.851555	-1.315251	1.222672
H	-5.038587	-1.254677	-2.285461
H	-5.100215	0.305237	-1.447353
H	-3.914747	0.042045	-2.732441
H	-2.752053	-3.147098	-1.945845
H	-1.544639	-1.934754	-2.359279
H	-1.408666	-2.866580	-0.843899
F	-0.023563	-0.000130	-3.102919

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