Supplementary information

Calcium catalysed nucleophilic fluorination

Job J.C. Struijs[1], Agamemnon E. Crumpton[1], Véronique Gouverneur[1,*], Simon Aldridge[1,*]

[1] *Chemistry Research Laboratory, Department of Chemistry, University of Oxford, Mansfield Road, Oxford, OX1 3TA (UK)*

** To whom correspondence should be addressed: veronique.gouverneur@chem.ox.ac.uk, simon.aldridge@chem.ox.ac.uk*

Table of Contents

1. Materials and methods 4
General considerations 4
Synthetic, spectroscopic, and analytical data 6
Synthesis of $^{Ar*}NONH_2$ 6
Synthesis of $^{Ar*}NONK_2$ 6
Synthesis of $(^{Ar*}NON)Mg(thf)_{2-x}(tol)_x$ 7
Synthesis of $(^{Ar*}NON)Ca(thf)_x$ (x=0: 1-□, x=1: 1-thf, x=2: 1-thf$_2$) 8
Synthesis of $(^{Ar*}NON)Sr$ 9
Synthesis of $(^{Ar*}NON)Ba$ 9
Synthesis of [TMA][$(^{Ar*}NON)CaF(thf)$] (2-TMA) 10
Synthesis of [PPh_4][$(^{Ar*}NON)CaF(thf)$] (2-PPh_4) 10
Synthesis of [TMA]$_2$[$(^{Ar*}NON)CaF_2$] (3-TMA$_2$) 11
Synthesis of [PPh_4]$_2$[$(^{Ar*}NON)CaF_2$] (3-(PPh_4)$_2$) 11
Synthesis of [TMA][$(^{Ar*}NON)CaCl(thf)$] (4-TMA) and [TMA]$_2$[$(^{Ar*}NON)CaCl_2$] (5-TMA$_2$) 12
Synthesis of [PPh_4][$(^{Ar*}NON)CaCl(thf)$] (4-PPh_4) 13
Synthesis of [K(2.2.2-crypt)][$(^{Ar*}NON)CaF$] (6-KCrypt) 13
Synthesis of [TMA]$_2$[$(^{Ar*}NON)CaFCl$] (7-TMA$_2$) 13
Synthesis of biphenyl-4-*d*$_2$-methanol 14
Synthesis of 4-(bromo-*d*$_2$-methyl)-biphenyl 14
2. Supplementary data 15
Isolation of terminal calcium fluoride complexes 15

Supplementary discussion 1 16
Supplementary discussion 2 19
Supplementary discussion 3 22
Reactivity of terminal calcium fluorides 23
Supplementary discussion 4 23
General procedure 24
Calcium-catalyzed fluorination using KF 32
Summary of initial experiments into the performance of other group 2 metals 32
Quantum chemical exploration of alternative mechanisms 36
General procedure 37
Hammett analysis and kinetic isotope effect study 40
Investigations into $[PPh_4]F$ as (in-situ generated) fluoride source 44
Catalyst decomposition studies 46
Analysis of the divergent reactivity for terminal calcium-fluoride complexes 48
3. NMR spectra of synthesized compounds 51
$^{Ar*}NONH_2$ 51
$^{Ar*}NONK_2$ 56
(^{Ar*}NON)Ca(thf) (1-thf) 64
(^{Ar*}NON)Ca (1-□) 69
(^{Ar*}NON)Mg(thf)(tol) 75
(^{Ar*}NON)Sr 81
(^{Ar*}NON)Ba 87
[TMA][(^{Ar*}NON)CaF(thf)] (2-TMA) 93
$[PPh_4]$[(^{Ar*}NON)CaF(thf)] (2-PPh_4) 100
$[TMA]_2$[(^{Ar*}NON)CaF_2] (3-TMA_2) 108
$[PPh_4]_2$[(Ar*NON)CaF_2] (3-$(PPh_4)_2$) 115
[TMA][(^{Ar*}NON)CaCl(thf)$_x$] (4-TMA) 121
$[PPh_4]$[(^{Ar*}NON)CaCl(thf)] (4-PPh_4) 127
[K(2.2.2-crypt)][(^{Ar*}NON)CaF] (6-KCrypt) 133
Biphenyl-4-d_2-methanol 134
4-(bromo-d_2-methyl)-biphenyl 136
4. X-ray crystallographic data 143
5. Quantum chemical computational details 148

General considerations.....148
Geometry optimisation and frequency calculations.....148
Single-point energy refinements.....148
Decomposition analyses.....148
Additional Analyses.....149
XYZ coordinates of optimized structures.....150
6. References.....235

1. Materials and methods

General considerations

All manipulations were carried out using standard Schlenk line or glovebox techniques under an atmosphere of argon or nitrogen, unless stated otherwise. Solvents were degassed by sparging with argon, dried by passing through a column of the appropriate drying agent, and stored over 3 Å or 4 Å molecular sieves (benzene, fluorobenzene, 1,2-difluorobenzene, dichloromethane, methanol, 2-methyltetrahydrofuran, and acetonitrile), over sodium (tetrahydrofuran), or over potassium (pentane, hexane, toluene, and diethyl ether). NMR spectra were measured in benzene-d_6 (dried over NaK and distilled under reduced pressure), tetrahydrofuran-d_8 (dried over molecular sieves), or acetonitrile-d_3 (dried over molecular sieves) which were stored over fresh molecular sieves in Teflon valve ampoules and degassed with 3 freeze-pump-thaw cycles. Anhydrous KF (Themo Scientific, 99%), TMAF (Sigma-Aldrich, 97%), and TMACl (TCI, 98%) were taken from freshly opened containers and dried under high vacuum (~$1x10^{-2}$ mbar) for 1 day at 80 °C. KH (Sigma-Aldrich, 30 wt% in mineral oil) was obtained by filtering the oil suspension over a fritted filter-Schlenk, washing the KH with minimal hexane, and drying the KH under vacuum, which was subsequently stored in a nitrogen-filled glovebox. 2.2.2-crypt (Fluorochem, 98%) was sublimed under vacuum and stored in a nitrogen-filled glovebox. 1-bromopentane (Fluorochem, 98%) and benzyl bromide (ThermoFisher, 98%) were syringed into ampoules with freshly dried molecular sieves and 3 freeze-pump-thaw cycles were performed. All other reagents were used (or cycled into a nitrogen-filled glovebox, indicated by *) as received: 9,9-dimethylxanthene (Apollo Scientific, 98%), tert-butyl chloride (Acros Organics, 99%), bromine (Fisher Scientific, 99.8%), diphenylmethanol (Fluorochem, 98%), p-toluidine (Sigma-Aldrich, 99%), $Pd(OAc)_2$* (Sigma-Aldrich, 98%), PCy_3* (Sigma-Aldrich, 99%), NaO^tBu* (TCI, 98%), anhydrous CaI_2* (Sigma-Aldrich, 99.999%), PPh_4Cl* (Fisher Scientific, 98%), PPh_4Br* (Alfa Aesar, 98%), $NaBF_4$ (Sigma-Aldrich, 98%), 1-adamantanecarbonyl chloride* (TCI, 97%), p-toluenesulfonyl chloride* (Fisher Scientific, >99%), Ph_3SiCl* (Sigma-Aldrich, 96%), PPh_3Cl_2* (Sigma-Aldrich, 95%), 4-(bromomethyl)biphenyl* (BLD Pharm, 98%), 4-(trifluoromethyl)benzyl bromide* (98%), 4-bromobenzyl bromide* (98%, Sigma-Aldrich), 4-methylbenzyl bromide* (Fluka, >97%), $LiAlD_4$* (Strem, >98 at% D), and biphenyl-4-carboxylic acid (Fluorochem, 97%). 4,5-Dibromo-2,7-di-tert-butyl-9,9-dimethylxanthene[1], $^{Dipp}NONH_2$[1], Ar^*NH_2[2], Ph_3SiN_3[3,4], and PPh_4F[5] were prepared according to (slightly modified) literature procedures.

NMR samples were prepared under argon or dinitrogen in 5 mm Wilmad 507-PP tubes fitted with J. Young Teflon valves. ^1H, ^{11}B, ^{19}F, ^{31}P, and $^{13}C\{^1H\}$ NMR spectra were recorded on a Bruker Avance III HD nanobay 400 MHz, Bruker Avance III 500 MHz or Bruker Avance III HD 600 MHz spectrometer at ambient temperature unless stated otherwise and referenced internally to residual protio-solvent (^1H) or solvent (^{13}C) resonances and are reported relative to tetramethylsilane (δ = 0 ppm). ^{11}B resonances are referenced externally to $BF_3{\cdot}OEt_2$ in $CDCl_3$, ^{19}F resonances externally to $CFCl_3$, in $CDCl_3$ and ^{31}P externally to 85% phosphoric acid in D_2O. Assignments were confirmed using ^1H-^1H COSY and NOESY/ROESY,

and ^{13}C-^{1}H HSQC and HMBC NMR correlation experiments. Chemical shifts are quoted in δ (ppm) and coupling constants in Hz. XA denotes the di-^{t}Bu-xanthene backbone, Ar* denotes the 2,6-dibenzhydryl-4-methylanilide moiety, and Ph denotes the phenyl rings of the Ar* moiety. *i*, *o*, *m*, *p* denote the *ipso*, *ortho*, *meta*, and *para* position of the aromatic rings, respectively. For 4-substituted biphenyl moieties, the substituted phenyl ring will be denoted by Ph_{sub} and the unsubstituted ring by Ph_{uns}, with the *ipso*-carbons being directly linked to each other. Elemental analyses were carried out by London Metropolitan University.

Single-crystal X-ray diffraction data were collected using either using an Oxford Diffraction/ Agilent SuperNova diffractometer (compound **1**-thf) or a Rigaku XtaLAB Synergy-DW VHF diffractometer equipped with a PhotonJet-R dual wavelength rotating anode and HyPix-Arc 150° detector (all other compounds). Crystals were selected under Paratone-N oil, mounted on Micromount loops and quench-cooled using an Oxford Cryosystems open flow N_2 cooling device. Data were collected at 100 K (or 200 K for **1**-thf$_2$ and 150K for **1**-thf) using mirror monochromated Cu Kα (λ = 1.5418 Å) or Mo Kα (λ = 0.71073 Å) radiation. Structure **1**-thf$_2$ was collected at a higher temperature (200 K) as the onset of a phase transition occurs proceeding to lower temperatures (at ca. 175 K). Data collected were processed using the CrysAlisPro package, including unit cell parameter refinement and inter-frame scaling (which was carried out using SCALE3 ABSPACK within CrysAlisPro). Equivalent reflections were merged and diffraction patterns processed with the CrysAlisPro suite. Structures were subsequently solved using SHELXT-2018 and refined on F^2 using the SHELXL 2018 package and the graphical interface Olex2. Finalized CIFs for all X-ray diffraction structures (2488575–2488587 and 2566165-2566166) have been deposited at the Cambridge Crystallographic Data Centre. These can be obtained free-of-charge via www.ccdc.cam.ac.uk/data_request/cif, by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

Synthetic, spectroscopic, and analytical data

Synthesis of $^{Ar*}NONH_2$

4,5-Dibromo-2,7-di-tert-butyl-9,9-dimethylxanthene (10.0 g, 20.8 mmol), Ar*NH_2 (18.3 g, 41.6 mmol), $Pd(OAc)_2$ (46.7 mg, 0.208 mmol), PCy_3 (117 mg, 0.416 mmol), and NaO^tBu (10.0 g, 104 mmol) were added to a Schlenk flask with stirrer bar, followed by 150 mL toluene. The suspension was heated to 100 °C and stirred for 16 h. After cooling down, the reaction was quenched by the addition of 300 mL H_2O. The aqueous layer was separated and extracted another 2x with 100 mL toluene. The combined organic fractions were dried with Na_2SO_4 and the crude product obtained by removal of the solvent under reduced pressure. The crude was dissolved in a minimal amount of hot toluene and let to crystalize upon cooling down. The product was filtered off, washed with a small amount of toluene, and dried under vacuum resulting in $^{Ar*}NONH_2$ (20.9 g, 84%).

^{1}H NMR (500 MHz, C_6D_6, 298 K) δ 7.22 (d, *J* = 7.4 Hz, 8H, Ph-*o*-C*H*), 7.12 (s, 4H, Ar*-*m*-C*H*), 7.08 (t, *J* = 7.6 Hz, 8H, Ph-*m*-C*H*), 7.01 (d, *J* = 7.5 Hz, 8H, Ph-*o*-C*H*), 6.98 (t, *J* = 7.4 Hz, 4H, Ph-*p*-C*H*), 6.94 (d, *J* = 2.2 Hz, 2H, XA-*p*-C*H*), 6.87 (t, *J* = 7.6 Hz, 8H, Ph-*m*-C*H*), 6.77 (t, *J* = 7.3 Hz, 2H, Ph-*p*-C*H*), 6.30 (d, *J* = 2.2 Hz, 2H, XA-*o*-C*H*), 6.05 (s, 4H, Ar*-C*H*Ph_2), 5.50 (s, 2H, N*H*), 1.86 (s, 6H, Ar*-CH_3), 1.70 (s, 6H, XA-C(CH_3)$_2$), 1.19 (s, 18H, XA-C(CH_3)$_3$) ppm.

^{13}C NMR (126 MHz, C_6D_6, 298 K) δ 145.5 (XA-*m*-*C*^{t}Bu), 145.0 (Ar*-*o*-*C*(CHPh$_2$)), 144.2 (Ph-*i*-*C*), 143.9 (Ph-*i*-*C*), 136.7 (XA-*o*-*C*O), 136.5 (Ar*-*i*-*C*N), 136.5 (Ar*-*p*-*C*), 135.5 (XA-*i*-*C*N), 130.3 (Ar*-*m*-*C*H), 130.1 (Ph-*o*-*C*H), 129.7 (XA-*m*-*C*(C(CH$_3$)$_2$)), 129.7 (Ph-*o*-*C*H), 128.7 (Ph-*m*-*C*H), 128.5 (Ph-*m*-*C*H), 126.6 (Ph-*p*-*C*H), 126.5 (Ph-*p*-*C*H), 112.3 (XA-*p*-*C*H), 108.7 (XA-*o*-*C*H), 52.2 (Ar*-*C*HPh$_2$), 35.0 (XA-*C*(CH$_3$)$_2$), 34.6 (XA-*C*(CH$_3$)$_3$), 32.6 (XA-C(*C*H$_3$)$_2$), 31.8 (XA-C(*C*H$_3$)$_3$), 21.4 (Ar*-*C*H$_3$) ppm.

HRMS (ESI) m/z calculated for $C_{89}H_{85}N_2O$ $[M+H]^+$ 1197.6656, found 1197.6689.

Synthesis of $^{Ar*}NONK_2$

$^{Ar*}NONH_2$ (4.00 g, 3.34 mmol) and KH (0.33 g, 8.35 mmol) were added to a Schlenk flask with stirrer bar. After the addition of 100 mL toluene, the suspension was stirred and heated at 80 °C for 16 h (note: hydrogen gas is formed). The solution was filtered into another Schlenk flask and the solvent was removed under reduced pressure, resulting in $^{Ar*}NONK_2$ in 96% yield (4.08 g). Single crystals suitable for Xray diffraction were obtained by slow evaporation from toluene.

^{1}H NMR (500 MHz, C_6D_6, 298 K) δ 7.22 – 7.12 (m, 16H, Ph-*o*-C*H,* Ph-*m*-C*H*), 7.08 – 7.02 (m, 4H, Ph-*p*-C*H*), 7.01 (s, 4H, Ar*-*m*-C*H*), 6.87 – 6.84 (m, 8H, Ph-*o*-C*H*), 6.81 (t, *J* = 7.6 Hz, 8H, Ph-*m*-C*H*), 6.75 (d, *J* = 2.3 Hz, 2H, XA-*p*-C*H*), 6.63 – 6.56 (m, 4H, Ph-*p*-C*H*), 6.59 (d, *J* = 2.7 Hz, 2H, XA-*o*-C*H*), 5.55 (s, 4H, Ar*-C*H*Ph_2), 1.97 (s, 6H, Ar*-CH_3), 1.90 (s, 6H, XA-C(CH_3)$_2$), 1.43 (s, 18H, XA-C(CH_3)$_3$) ppm.

^{13}C NMR (126 MHz, C_6D_6, 298 K) δ 153.7 (Ar*-*i*-*C*N), 148.5 (XA-*i*-*C*N), 147.0 (XA-*m*-*C*^{t}Bu), 146.8 (Ph-*i*-*C*), 145.8 (Ph-*i*-*C*), 138.4 (Ar*-*o*-*C*(CHPh$_2$)), 138.1 (XA-*o*-*C*O), 133.3 (XA-*m*-

C(C(CH$_3$)$_2$)), 130.6 (Ar*-*m*-*C*H), 130.3 (Ph-*o*-*C*H), 129.6 (Ph-*o*-*C*H), 128.7 (Ph-*m*-*C*H), 128.5 (Ph-*m*-*C*H), 127.1 (Ar*-*p*-*C*), 126.5 (Ph-*p*-*C*H), 126.3 (Ph-*p*-*C*H), 111.0 (XA-*o*-*C*H), 102.6 (XA-*p*-*C*H), 52.2 (Ar*-*C*HPh$_2$), 35.8 (XA-*C*(CH$_3$)$_2$), 35.1 (XA-*C*(CH$_3$)$_3$), 32.3 (XA-C(*C*H$_3$)$_3$), 30.0 (XA-C(*C*H$_3$)$_2$), 21.3 (Ar*-*C*H$_3$) ppm.

Elemental analysis: anal. calc. for $C_{96}H_{90}K_2N_2O$: C 84.41%, H 6.64%, N 2.05%, found: C 84.04%, H 6.85%, N 1.98%.

Synthesis of (^{Ar*}NON)Mg(thf)$_{2-x}$(tol)$_x$

^{Ar*}NONK$_2$ (683 mg, 0.50 mmol) and MgI$_2$ (139 mg, 0.50 mmol. *Nota bene*: a large excess of MgI$_2$ was found to lead to separation difficulties) were added to a Schlenk flask with stirrer bar followed by 20 mL of thf. The reaction mixture was stirred at 60 °C for 24 h, after which the solvent was completely removed under reduced pressure. The resulting solids were then extracted with toluene (3x10 mL, x=1) and filtered into another Schlenk flask. The toluene solution was then concentrated under reduced pressure and the flask was moved to the freezer to result in crystalline product (addition of small portions of hexane can assist the crystallization if needed). The mother liquor was removed (and resubjected to crystallization) and (^{Ar*}NON)Mg(thf)(tol) was dried under vacuum (452 mg, 65%). Alternatively, an extraction with DCM (3x25 mL, for x=0) can be performed and, further following the analogous synthesis for all other (^{Ar*}NON)AE complexes, results in the formation of (^{Ar*}NON)Mg(thf)$_2$, yet in variable and lower yields. Upon dissolution of (^{Ar*}NON)Mg(thf)(tol) in thf(-d$_8$), identical NMR spectra are obtained as for (^{Ar*}NON)Mg(thf)$_2$ and evaporation yields (^{Ar*}NON)Mg(thf)$_2$ in a quantitative conversion.

^{1}H NMR (500 MHz, thf-d$_8$, 298 K) δ 7.18 (t, *J* = 7.5 Hz, 2H, tol-*m*-C*H*), 7.12 (s, 4H, Ar*-*m*-C*H*), 7.10 – 7.00 (m, 3H, tol-*o*-C*H,* tol-*p*-C*H*), 6.95 – 6.88 (m, 20H, Ph-*o*-C*H,* Ph-*m*-C*H,* Ph-*p*-C*H*), 6.86 – 6.78 (m, 20H, Ph-*o*-C*H,* Ph-*m*-C*H,* Ph-*p*-C*H*), 6.22 (d, *J* = 2.0 Hz, 2H, XA-*p*-C*H*), 6.12 (s, 4H, Ar*-*m*-C*H*), 4.72 (d, *J* = 2.0 Hz, 2H, XA-*o*-C*H*), 3.63 – 3.60 (m, 4H, thf-2,5-C*H*$_2$), 2.31 (s, 3H, tol-C*H*$_3$), 2.20 (s, 6H, Ar*-C*H*$_3$), 1.79 – 1.75 (m, 4H, thf-3,4-C*H*$_2$), 1.69 (s, 6H, XA-C(C*H*$_3$)$_2$), 0.66 (s, 18H, XA-C(C*H*$_3$)$_3$) ppm.

^{13}C NMR (126 MHz, thf-d$_8$, 298 K) δ 152.9 (Ar*-*i*-*C*N), 148.1 (XA-*i*-*C*N), 147.7 (Ph-*i*-*C*), 146.0 (Ph-*i*-*C*), 145.7 (XA-*m*-*C*^{t}Bu), 142.5 (Ar*-*o*-*C*(CHPh$_2$)), 138.6 (tol-*i*-*C*), 136.8 (XA-*o*-*C*O), 131.2 (Ar*-*m*-*C*H), 131.1 (Ar*-*p*-*C*), 131.1 (Ph-*o*-*C*H), 130.5 (Ph-*o*-*C*H), 129.8 (tol-*o*-*C*H), 129.3 (XA-*m*-*C*(C(CH$_3$)$_2$)), 129.1 (tol-*m*-*C*H), 128.6 (Ph-*m*-*C*H), 128.4 (Ph-*m*-*C*H), 126.2 (Ph-*p*-*C*H), 126.2 (tol-*p*-*C*H), 126.1 (Ph-*p*-*C*H), 111.6 (XA-*o*-*C*H), 104.9 (XA-*p*-*C*H), 68.4 (thf-2,5-*C*H$_2$), 51.8 (Ar*-*C*HPh$_2$), 35.7 (XA-*C*(CH$_3$)$_2$), 34.9 (XA-*C*(CH$_3$)$_3$), 32.0 (XA-C(*C*H$_3$)$_3$), 31.8 (XA-C(*C*H$_3$)$_2$), 26.6 (thf-3,4-*C*H$_2$), 21.7 (Ar*-*C*H$_3$), 21.7 (tol-C(*C*H$_3$)) ppm.

Elemental analysis: anal. calc. for $C_{97}H_{98}MgN_2O_3$: C 85.41%, H 7.24%, N 2.05%, found: C 85.65%, H 7.18%, N 1.96%.

Synthesis of (^{Ar*}NON)Ca(thf)$_x$ (x=0: 1-□, x=1: 1-thf, x=2: 1-thf$_2$)

^{Ar*}NONK$_2$ (683 mg, 0.50 mmol) and CaI$_2$ (294 mg, 1.00 mmol) were added to a Schlenk flask with stirrer bar followed by 20 mL of thf. The reaction mixture was stirred at 50 °C for 20 h, after which the solvent was completely removed under reduced pressure. The resulting solids were then extracted with DCM (3x20mL) and filtered into another Schlenk flask (an extraction with toluene, affording x=1, can also be done but leaves traces of KI in product). An equal portion of hexane was layered onto the DCM solution and the flask was moved to the freezer to result in crystalline product. The mother liquor was removed (and resubjected to crystallization) and the crystals of **1** dried under vacuum (450 mg, 69%). In order to remove all traces of DCM (shown to cause side reactivity in future reactions), **1** can be dissolved in e.g. minimal toluene (for x=0) or thf (for x=1) and evaporated to dryness. Single crystals suitable for single crystal XRD of the bis-thf complex 1-thf$_2$ (x=2) were grown by cooling down a hot saturated solution of (^{Ar*}NON)Ca(thf)$_x$ in thf.

(^{Ar*}NON)Ca(thf)

^{1}H NMR (400 MHz, C_6D_6, 298 K) δ 7.24 – 7.09 (m, 20H, Ph-*o*-C*H,* Ph-*m*-C*H,* Ar*-*m*-C*H*), 7.06 – 7.00 (m, 4H, Ph-*p*-C*H*), 7.00 – 6.96 (m, 8H, Ph-*o*-C*H*), 6.79 (d, J = 2.2 Hz, 2H, XA-*p*-C*H*), 6.73 (t, J = 7.5 Hz, 8H, Ph-*m*-C*H*), 6.68 – 6.61 (m, 4H, Ph-*p*-C*H*), 6.21 (d, J = 2.2 Hz, 2H, XA-*o*-C*H*), 5.94 (s, 4H, Ar*-C*H*Ph$_2$), 3.17 (s, 4H, thf-2,5-C*H*$_2$), 2.06 (s, 6H, Ar*-C*H*$_3$), 1.96 (s, 6H, XA-C(C*H*$_3$)$_2$), 1.33 (s, 18H, XA-C(C*H*$_3$)$_3$), 1.24 (s, 4H, thf-3,4-C*H*$_2$) ppm.

^{13}C NMR (101 MHz, C_6D_6, 298 K) δ 150.6 (Ar*-*i*-*C*N), 147.8 (Ph-*i*-*C*), 146.8 (XA-*i*-*C*N), 146.6 (XA-*m*-*C*^{t}Bu), 145.2 (Ph-*i*-*C*), 141.4 (Ar*-*o*-*C*(CHPh$_2$)), 138.3 (XA-*o*-*C*O), 130.2 (Ar*-*p*-*C*), 130.1 (Ph-*o*-*C*H), 129.9 (Ar*-*m*-*C*H), 129.9 (Ph-*o*-*C*H), 129.3 (XA-*m*-*C*(C(CH$_3$)$_2$)), 129.0 (Ph-*m*-*C*H), 128.5 (Ph-*m*-*C*H), 126.6 (Ph-*p*-*C*H), 126.3 (Ph-*p*-*C*H), 109.3 (XA-*o*-*C*H), 105.8 (XA-*p*-*C*H), 68.4 (thf-2,5-*C*H$_2$), 51.8 (Ar*-*C*HPh$_2$), 35.1 (XA-*C*(CH$_3$)$_2$), 34.9 (XA-*C*(CH$_3$)$_3$), 32.7 (XA-C(*C*H$_3$)$_2$), 32.2 (XA-C(*C*H$_3$)$_3$), 25.5 (thf-3,4-*C*H$_2$), 21.5 (Ar*-*C*H$_3$) ppm.

Elemental analysis: anal. calc. for $C_{97}H_{98}CaN_2O_3$: C 84.43%, H 7.16%, N 2.03%, found: C 84.09%, H 7.06%, N 1.90%.

(^{Ar*}NON)Ca

^{1}H NMR (500 MHz, C_6D_6, 298 K) δ 7.18 (s, 4H, Ar*-*m*-C*H*), 7.15 – 7.13 (m, 16H, Ph-*o*-C*H,* Ph-*m*-C*H*), 7.06 – 7.01 (m, 4H, Ph-*p*-C*H*), 6.90 – 6.82 (m, 8H, Ph-*o*-C*H*), 6.83 (d, *J* = 2.2 Hz, 2H, XA-*p*-C*H*), 6.59 (t, *J* = 7.4 Hz, 8H, Ph-*m*-C*H*), 6.56 – 6.51 (m, 4H, Ph-*p*-C*H*), 6.50 (d, *J* = 2.2 Hz, 2H, XA-*o*-C*H*), 5.81 (s, 4H, Ar*-C*H*Ph$_2$), 2.10 (s, 6H, Ar*-C*H*$_3$), 1.97 (s, 6H, XA-C(C*H*$_3$)$_2$), 1.39 (s, 18H, XA-C(C*H*$_3$)$_3$) ppm.

^{13}C NMR (126 MHz, C_6D_6, 298 K) δ 150.3 (Ar*-*i*-*C*N), 147.9 (Ph-*i*-*C*), 147.1 (XA-*i*-*C*N), 147.0 (XA-*m*-*C*^{t}Bu), 145.2 (Ph-*i*-*C*), 141.2 (Ar*-*o*-*C*(CHPh$_2$)), 138.9 (XA-*o*-*C*O), 130.3 (Ar*-*p*-*C*), 130.0 (Ph-*o*-*C*H), 130.0 (Ph-*o*-*C*H), 129.4 (Ph-*m*-*C*H), 129.3 (XA-*m*-*C*(C(CH$_3$)$_2$)), 128.4, 128.4 (Ph-*m*-*C*H), 126.8 (Ar*-*m*-*C*H), 126.3 (Ph-*p*-*C*H), 125.7 (Ph-*p*-*C*H), 108.9 (XA-*o*-*C*H), 105.6 (XA-*p*-*C*H), 51.9 (Ar*-*C*HPh$_2$), 35.3 (XA-*C*(CH$_3$)$_2$), 35.0 (XA-*C*(CH$_3$)$_3$), 32.2 (XA-C(*C*H$_3$)$_3$), 32.0 (XA-C(*C*H$_3$)$_2$), 21.5 (Ar*-*C*H$_3$) ppm.

Elemental analysis: anal. calc. for $C_{110}H_{106}CaN_2O$: C 87.37%, H 7.07%, N 1.85%, found: C 87.43%, H 7.16%, N 1.87%.

Synthesis of (^{Ar*}NON)Sr

$^{Ar*}NONK_2$ (683 mg, 0.50 mmol) and SrI_2 (341 mg, 1.00 mmol) were added to a Schlenk flask with stirrer bar followed by 20 mL of thf. The reaction mixture was stirred at 50 °C for 16 h, after which the solvent was completely removed under reduced pressure. The resulting solids were then extracted with DCM (3x25 mL) and filtered into another Schlenk flask. A double portion of hexane (150 ml) was layered onto the DCM solution and the flask was moved to the freezer to result in crystalline product. The mother liquor was removed (and resubjected to crystallization) and the crystals of (^{Ar*}NON)Sr dried under vacuum (394 mg, 61%). In order to remove all traces of DCM, (^{Ar*}NON)Sr can be dissolved in minimal toluene and evaporated to dryness.

^{1}H NMR (500 MHz, thf-d_8, 298 K) δ 7.07 – 7.03 (m, 8H, Ph-*m*-C*H*), 7.02 – 6.98 (m, 4H, Ph-*p*-C*H*), 6.98 – 6.96 (m, 16H, Ph-*m*-C*H,* Ph-*o*-C*H*), 6.96 – 6.93 (m, 8H, Ph-*o*-C*H*), 6.91 (s, 4H, Ar*-*m*-C*H*), 6.83 – 6.77 (m, 4H, Ph-*p*-C*H*), 6.37 (d, *J* = 2.3 Hz, 2H, XA-*p*-C*H*), 5.86 (s, 4H, Ar*-C*H*Ph_2), 5.60 (d, *J* = 2.2 Hz, 2H, XA-*o*-C*H*), 2.14 (s, 6H, Ar*-CH_3), 1.73 (s, 6H, XA-C(CH_3)$_2$), 0.97 (s, 18H, XA-C(CH_3)$_3$) ppm.

^{13}C NMR (126 MHz, thf-d_8, 298 K) δ 153.0 (Ar*-*i*-*C*N), 149.1 (XA-*i*-*C*N), 147.4 (Ph-*i*-*C*), 146.9 (Ph-*i*-*C*), 146.1 (XA-*m*-*C*^{t}Bu), 139.5 (XA-*o*-*C*O), 130.9 (Ar*-*p*-*C*), 130.7 (Ph-*o*-*C*H), 130.7 (Ph-*o*-*C*H), 129.8 (XA-*m*-*C*(C$(CH_3)_2$)), 129.2 (Ph-*m*-*C*H), 128.6 (Ph-*m*-*C*H), 127.0 (Ph-*p*-*C*H), 126.2 (Ph-*p*-*C*H), 111.4 (XA-*o*-*C*H), 105.2 (XA-*p*-*C*H), 51.9 (Ar*-*C*HPh_2), 35.6 (XA-*C*$(CH_3)_2$), 35.1 (XA-*C*$(CH_3)_3$), 33.2 (XA-C(*C*H_3)$_2$), 32.3 (XA-C(*C*H_3)$_3$), 21.6 (Ar*-*C*H_3) ppm.

Elemental analysis: anal. calc. for $C_{96}H_{90}SrN_2O$: C 83.83%, H 6.60%, N 2.04%, found: C 83.46%, H 6.72%, N 2.06%.

Synthesis of (^{Ar*}NON)Ba

$^{Ar*}NONK_2$ (683 mg, 0.50 mmol) and BaI_2 (391 mg, 1.00 mmol) were added to a Schlenk flask with stirrer bar followed by 20 mL of thf. The reaction mixture was stirred at 50 °C for 16 h, after which the solvent was completely removed under reduced pressure. The resulting solids were then extracted with DCM (3x15 mL) and filtered into another Schlenk flask. A double portion of hexane was layered onto the DCM solution and the flask was moved to the freezer to result in crystalline product. The mother liquor was removed (and resubjected to crystallization) and the crystals of (^{Ar*}NON)Ba dried under vacuum (481 mg, 72%). In order to remove all traces of DCM, (^{Ar*}NON)Ba can be dissolved in minimal toluene and evaporated to dryness.

^{1}H NMR (500 MHz, thf-d_8, 298 K) δ 7.09 – 7.04 (m, 16H, Ph-*m*-C*H*), 7.03 – 6.99 (m, 12H, Ph-*o*-C*H,* Ph-*p*-C*H*), 6.94 (dd, *J* = 6.9, 1.8 Hz, 8H, Ph-*o*-C*H*), 6.84 (s, 4H, Ar*-*m*-C*H*), 6.76 (tt, *J* = 7.3, 1.5 Hz, 4H, Ph-*p*-C*H*), 6.36 (d, *J* = 2.3 Hz, 2H, XA-*p*-C*H*), 5.80 (s, 4H, Ar*-C*H*Ph_2), 5.53 (d, *J*

= 2.3 Hz, 2H, XA-*o*-C*H*), 2.12 (s, 6H, Ar*-CH_3), 1.75 (s, 6H, XA-C(CH_3)$_2$), 0.99 (s, 18H, XA-C(CH_3)$_3$) ppm.

^{13}C NMR (126 MHz, thf-d$_8$, 298 K) δ 151.6 (Ar*-*i*-*C*N), 148.7 (Ph-*i*-*C*), 148.3 (XA-*i*-*C*N), 146.4 (Ph-*i*-*C*), 145.8 (XA-*m*-*C*^{t}Bu), 141.9 (Ar*-*o*-*C*(CHPh$_2$)), 140.4 (XA-*o*-*C*O), 130.7 (Ph-*o*-*C*H), 130.6 (Ar*-*m*-*C*H), 130.5 (Ar*-*p*-*C*), 129.5 (Ph-*m*-*C*H), 129.5 (XA-*m*-*C*(C(CH$_3$)$_2$)), 128.7 (Ph-*m*-*C*H), 127.2 (Ph-*p*-*C*H), 126.4 (Ph-*p*-*C*H), 110.1 (XA-*o*-*C*H), 105.5 (XA-*p*-*C*H), 52.0 (Ar*-*C*HPh$_2$), 35.4 (XA-*C*(CH$_3$)$_2$), 35.0 (XA-*C*(CH$_3$)$_3$), 33.8 (XA-C(*C*H$_3$)$_2$), 32.3 (XA-C(*C*H$_3$)$_3$), 21.6 (Ar*-*C*H$_3$) ppm.

Elemental analysis: anal. calc. for $C_{103}H_{98}BaN_2O$: C 81.54%, H 6.51%, N 1.85%, found: C 81.62%, H 6.53%, N 1.87%.

Synthesis of [TMA][(^{Ar*}NON)CaF(thf)] (2-TMA)

(^{Ar*}NON)Ca (13.3 mg, 0.01 mmol), TMAF (0.9 mg, 0.01 mmol) and 0.5 mL thf-d$_8$ were added to a J. Young NMR tube. The solution sonicated and heated (also proceeds at room temperature) to speed up the reaction until full conversion to **2**-TMA was observed by ^{1}H NMR (~30 min). Single crystals of [TMA][(^{Ar*}NON)CaF(thf)] were never obtained by all attempted crystallization methods; instead all formed crystals yielded [TMA]$_2$[(^{Ar*}NON)CaF$_2$].

^{1}H NMR (500 MHz, thf-d$_8$, 298 K) δ 7.23 (d, *J* = 7.6 Hz, 8H, Ph-*o*-C*H*), 7.07 (d, *J* = 7.4 Hz, 8H, Ph-*o*-C*H*), 6.99 (t, *J* = 7.3 Hz, 8H, Ph-*m*-C*H*), 6.97 (t, *J* = 7.7 Hz, 8H, Ph-*m*-C*H*), 6.94 – 6.89 (m, 4H, Ph-*p*-C*H*), 6.88 (s, 4H, Ar*-*m*-C*H*), 6.82 (t, *J* = 6.8 Hz, 4H, Ph-*p*-C*H*), 6.42 (s, 4H, Ar*-C*H*Ph$_2$), 6.06 (d, *J* = 2.3 Hz, 2H, XA-*p*-C*H*), 5.22 (d, *J* = 2.2 Hz, 2H, XA-*o*-C*H*), 2.69 (s, 12H, $^+$N(C*H*$_3$)$_4$), 2.14 (s, 6H, Ar*-C*H*$_3$), 1.67 (s, 6H, XA-C(C*H*$_3$)$_2$), 0.80 (s, 18H, XA-C(C*H*$_3$)$_3$) ppm.

^{19}F NMR (470 MHz, thf-d$_8$, 298 K) δ -55.8 (Ca*F*) ppm.

^{13}C NMR (126 MHz, thf-d$_8$, 298 K) δ 153.5 (Ar*-*i*-*C*N), 149.5 (XA-*i*-*C*N), 148.2 (Ph-*i*-*C*), 147.2 (Ph-*i*-*C*), 145.4 (XA-*m*-*C*^{t}Bu), 142.0 (Ar*-*o*-*C*(CHPh$_2$)), 138.7 (XA-*o*-*C*O), 131.1 (Ph-*o*-*C*H), 130.9 (Ph-*o*-*C*H), 130.6 (Ar*-*m*-*C*H), 129.8 (Ar*-*p*-*C*), 129.1 (XA-*m*-*C*(C(CH$_3$)$_2$)), 128.6 (Ph-*m*-*C*H), 128.3 (Ph-*m*-*C*H), 126.0 (Ph-*p*-*C*H), 125.7 (Ph-*p*-*C*H), 110.5 (XA-*o*-*C*H), 102.5 (XA-*p*-*C*H), 55.5 ($^+$N(*C*H$_3$)$_4$), 51.5 (Ar*-*C*HPh$_2$), 35.1 (XA-*C*(CH$_3$)$_2$), 34.9 (XA-*C*(CH$_3$)$_3$), 32.2 (XA-C(*C*H$_3$)$_3$), 32.0 (XA-C(*C*H$_3$)$_2$), 21.7 (Ar*-*C*H$_3$) ppm.

Synthesis of [PPh$_4$][(^{Ar*}NON)CaF(thf)] (2-PPh$_4$)

(^{Ar*}NON)Ca (12.4 mg, 0.01 mmol) and PPh$_4$F (3.6 mg, 0.01 mmol) and 0.5 mL thf-d$_8$ were added to a J. Young NMR tube. The solution was sonicated briefly resulting in an immediate full conversion to **2**-PPh$_4$ as observed by ^{1}H NMR. The solution was then filtered and layered with an equal amount of hexane. Red crystals of **2**-PPh$_4$ formed over the course of 2 weeks, suitable for single crystal diffraction.

^{1}H NMR (400 MHz, thf-d$_8$, 298 K) δ 7.81 (dq, *J* = 5.4, 3.8 Hz, 4H, $^+$PPh$_4$-*p*-C*H*), 7.73 – 7.57 (m, 16H, $^+$PPh$_4$-*o*-C*H*, $^+$PPh$_4$-*m*-C*H*), 7.25 (d, *J* = 7.6 Hz, 8H, Ph-*o*-C*H*), 7.02 (d, *J* = 7.3 Hz, 8H, Ph-*o*-C*H*), 6.92 – 6.86 (m, 8H, Ph-*m*-C*H*), 6.86 – 6.81 (m, 4H, Ph-*p*-C*H*), 6.78 (t, *J* = 7.6 Hz, 8H, Ph-*m*-C*H*), 6.70 (s, 4H, Ar*-*m*-C*H*), 6.67 (t, *J* = 7.4 Hz, 4H, Ph-*p*-C*H*), 6.34 (s, 4H, Ar*-C*H*Ph$_2$), 5.92

(d, *J* = 2.3 Hz, 2H, XA-*p*-C*H*), 5.02 (d, *J* = 2.2 Hz, 2H, XA-*o*-C*H*), 2.00 (s, 6H, Ar*-CH_3), 1.57 (s, 6H, XA-C(CH_3)$_2$), 0.75 (s, 18H, XA-C(CH_3)$_3$) ppm.

^{19}F NMR (470 MHz, thf-d$_8$, 298 K) δ -64.3 (Ca*F*) ppm.

^{31}P NMR (202 MHz, thf-d$_8$, 298 K) δ 20.8 ([*P*Ph$_4$]$^+$) ppm.

^{13}C NMR (126 MHz, thf-d$_8$, 298 K) δ 153.4 (Ar*-*i*-*C*N), 149.3 (Ph-*i*-*C*), 148.8 (XA-*i*-*C*N), 146.3 (Ph-*i*-*C*), 144.2 (XA-*m*-*C*^{t}Bu), 142.7 (Ar*-*o*-*C*(CHPh$_2$)), 138.5 (XA-*o*-*C*O), 136.8 (d, *J* = 3.1 Hz, $^+$PPh$_4$-*p*-*C*H), 135.7 (d, *J* = 10.5 Hz, $^+$PPh$_4$-*m*-*C*H), 131.7 (d, *J* = 12.7 Hz, $^+$PPh$_4$-*o*-*C*H), 131.1 (Ph-*o*-*C*H), 130.1 (Ar*-*m*-*C*H), 128.3 (Ph-*m*-*C*H), 128.2 (Ph-*m*-*C*H), 127.9 (Ar*-*p*-*C*), 127.7 (XA-*m*-*C*(C(CH$_3$)$_2$)), 125.6 (Ph-*p*-*C*H), 125.4 (Ph-*p*-*C*H), 119.1 (d, *J* = 89.2 Hz, $^+$PPh$_4$-*i*-*C*H), 109.1 (XA-*o*-*C*H), 103.2 (XA-*p*-*C*H), 52.1 (Ar*-*C*HPh$_2$), 35.0 (XA-*C*(CH$_3$)$_2$), 34.7 (XA-C(*C*H$_3$)$_3$), 33.7 (XA-C(*C*H$_3$)$_2$), 32.4 (XA-C(*C*H$_3$)$_3$), 21.9 (Ar*-*C*H$_3$) ppm.

Elemental analysis: anal. calc. for $C_{123}H_{124}CaFN_2O_2P$: C 84.30%, H 7.13%, N 1.60%, found: C 83.98%, H 7.42%, N 1.42%.

Synthesis of [TMA]$_2$[(^{Ar*}NON)CaF$_2$] (3-TMA$_2$)

(^{Ar*}NON)Ca (18.5 mg, 0.015 mmol), TMAF (2.8 mg, 0.030 mmol) and 0.5 mL thf-d$_8$ were added to a J. Young NMR tube. The solution was heated at 80 °C until full conversion to **3**-TMA$_2$ was observed by ^{1}H NMR (~5 min). Single crystals suitable for Xray diffraction of [TMA]$_2$[(^{Ar*}NON)CaF$_2$] were obtained by placing the NMR tube in an 80 °C oil bath overnight, yielding crystals just above the liquid-gas interface.

^{1}H NMR (500 MHz, thf-d$_8$, 298 K) δ 7.50 (d, *J* = 7.4 Hz, 8H, Ph-*o*-C*H*), 7.17 (d, *J* = 7.6 Hz, 8H, Ph-*o*-C*H*), 7.00 – 6.92 (m, 16H, Ph-*m*-C*H*), 6.90 – 6.85 (m, 4H, Ph-*p*-C*H*), 6.84 – 6.80 (m, 8H, Ph-*m*-C*H,* Ar*-C*H*Ph$_2$), 6.79 (s, 4H, Ar*-*m*-C*H*), 5.77 (d, *J* = 2.3 Hz, 2H, XA-*p*-C*H*), 5.07 (d, *J* = 2.3 Hz, 2H, XA-*o*-C*H*), 2.58 (s, 24H, $^+$N(C*H*$_3$)$_4$), 2.12 (s, Ar*-C*H*$_3$), 1.54 (s, 6H, XA-C(C*H*$_3$)$_2$), 0.64 (s, 18H, XA-C(C*H*$_3$)$_3$) ppm.

^{19}F NMR (377 MHz, thf-d$_8$, 298 K) δ -72.8 (Ca*F*$_2$) ppm.

^{13}C NMR (126 MHz, thf-d$_8$, 298 K) δ 154.9 (Ar*-*i*-*C*N), 150.3 (Ph-*i*-*C*), 149.9 (XA-*i*-*C*N), 147.4 (Ph-*i*-*C*), 144.8 (XA-*m*-*C*^{t}Bu), 141.5 (Ar*-*o*-*C*(CHPh$_2$)), 139.4 (XA-*o*-*C*O), 131.7 (Ph-*o*-*C*H), 131.2 (Ph-*o*-*C*H), 130.5 (Ar*-*m*-*C*H), 128.2 (Ph-*m*-*C*H), 128.1 (Ph-*m*-*C*H), 126.7 (Ar*-*p*-*C*), 126.2 (XA-*m*-*C*(C(CH$_3$)$_2$)), 125.3 (Ph-*p*-*C*H), 125.2 (Ph-*p*-*C*H), 110.4 (XA-*o*-*C*H), 100.5 (XA-*p*-*C*H), 55.4 ($^+$N(*C*H$_3$)$_4$), 51.4 (Ar*-*C*HPh$_2$), 34.9 (XA-*C*(CH$_3$)$_2$), 34.6 (XA-*C*(CH$_3$)$_3$), 32.2 (XA-C(*C*H$_3$)$_3$), 32.0 (XA-C(*C*H$_3$)$_2$), 21.8 (Ar*-*C*H$_3$) ppm.

Synthesis of [PPh$_4$]$_2$[(^{Ar*}NON)CaF$_2$] (3-(PPh$_4$)$_2$)

(^{Ar*}NON)Ca (12.4 mg, 0.01 mmol) and PPh$_4$F (7.2 mg, 0.02 mmol) and 0.5 mL MeCN-d$_3$ were added to a J. Young NMR tube. The solution was sonicated until full conversion to **3**-(PPh$_4$)$_2$ was observed by ^{1}H NMR. The solid that is formed in the reaction (**3**-(PPh$_4$)$_2$ is not very soluble even in MeCN) was washed with MeCN-d$_3$ two times, after which clean **3**-(PPh$_4$)$_2$

was obtained. Note: as **3**-$(PPh_4)_2$ is unstable in MeCN, the NMR characterization was performed as soon as possible but minor decomposition can be observed (all other solvents tested displayed a solubility unsuitable for NMR characterization of **3**-$(PPh_4)_2$). Red crystals suitable for single crystal diffraction were obtained by slow evaporation from a saturated solution of **3**-$(PPh_4)_2$ in o-DFB.

^{1}H NMR (500 MHz, MeCN-d_3, 298 K) δ 7.92 – 7.78 (m, 8H, $^+$PPh$_4$-*p*-C*H*), 7.76 – 7.50 (m, 32H, $^+$PPh$_4$-*o*-C*H,* $^+$PPh$_4$-m-C*H*), 7.49 (d, J = 6.5 Hz, 8H, Ph-*o*-C*H*), 7.11 – 7.06 (m, 8H, Ph-*o*-C*H*), 6.99 (t, J = 7.6 Hz, 8H, Ph-*m*-C*H*), 6.97 (t, J = 7.5 Hz, 8H, Ph-*m*-C*H*), 6.88 (t, J = 7.3 Hz, 8H, Ph-*p*-C*H*), 6.65 (s, 4H, Ar*-C*H*Ph$_2$), 6.63 (s, 4H, Ar*-*m*-C*H*), 5.66 (d, J = 2.3 Hz, 2H, XA-*p*-C*H*), 4.64 (d, J = 2.3 Hz, 2H, XA-*o*-C*H*), 2.07 (s, 6H, Ar*-C*H*$_3$), 1.48 (s, 6H, XA-C(C*H*$_3$)$_2$), 0.53 (s, 18H, XA-C(C*H*$_3$)$_3$) ppm.

^{19}F NMR (470 MHz, MeCN-d_3, 298 K) δ -71.3 (Ca*F*$_2$) ppm.

^{31}P NMR (202 MHz, MeCN-d_3, 298 K) δ 17.5 ([*P*Ph$_4$]$^+$) ppm.

^{13}C NMR (126 MHz, MeCN-d_3, 298 K) δ 154.5 (Ar*-*i*-*C*N), 149.9 (Ph-*i*-*C*), 149.9 (XA-*i*-*C*N), 146.3 (Ph-*i*-*C*), 143.7 (XA-*m*-*C*^{t}Bu), 142.4 (Ar*-*o*-*C*(CHPh$_2$)), 138.5 (XA-*o*-*C*O), 133.8 (d, J = 9.7 Hz, $^+$PPh$_4$-*m*-*C*H), 133.3 (d, J = 2.7 Hz, $^+$PPh$_4$-*p*-*C*H), 131.2 (Ph-*o*-*C*H), 131.1 (Ph-*o*-*C*H), 130.8 (Ar*-*p*-*C*), 130.0 (Ar*-*m*-*C*H), 129.7 (d, J = 12.1 Hz, $^+$PPh$_4$-*o*-*C*H), 128.3 (Ph-*m*-*C*H), 128.2 (Ph-*m*-*C*H), 126.3 (XA-*m*-*C*(C(CH$_3$)$_2$)), 125.5 (Ph-*p*-*C*H), 125.3 (Ph-*p*-*C*H), 120.3 (d, J = 83.7 Hz, $^+$PPh$_4$-*i*-*C*H), 108.9 (XA-*o*-*C*H), 101.2 (XA-*p*-*C*H), 51.2 (Ar*-*C*HPh$_2$), 34.7 (XA-*C*(CH$_3$)$_2$), 34.2 (XA-*C*(CH$_3$)$_3$), 33.3 (XA-*C*(CH$_3$)$_2$), 31.8 (XA-*C*(CH$_3$)$_3$), 21.5 (Ar*-*C*H$_3$) ppm.

Synthesis of [TMA][(^{Ar*}NON)CaCl(thf)] (4-TMA) and [TMA]$_2$[(^{Ar*}NON)CaCl$_2$] (5-TMA$_2$)
(^{Ar*}NON)Ca(thf) (9.8 mg, 7.5 µmol), TMACl (0.8 mg, 7.5 µmol) and 0.5 mL thf-d_8 were added to a J. Young NMR tube. The solution was left at room temperature (or sonicated or heated to speed up the reaction) until full conversion to **4**-TMA was observed by ^{1}H NMR (~4 days). Heating a 15 µmol scale reaction (in 0.5 mL) in a J. Young NMR tube at 80 °C for 3 days yielded single crystals of [TMA]$_2$[(^{Ar*}NON)CaCl$_2$] (**5**-TMA$_2$). Single crystals of [TMA][(^{Ar*}NON)CaCl(thf)] were never obtained by all attempted crystallization methods.

^{1}H NMR (500 MHz, thf-d_8, 298 K) δ 7.26 – 7.17 (m, 8H, Ph-*o*-C*H*), 7.09 – 7.00 (m, 8H, Ph-*o*-C*H*), 6.93 (t, *J* = 6.7 Hz, 8H, Ph-*m*-C*H*), 6.91 (t, *J* = 6.0 Hz, 8H, Ph-*m*-C*H*), 6.90 – 6.83 (m, 4H, Ph-*p*-C*H*), 6.89 – 6.82 (m, 4H, Ph-*p*-C*H*), 6.75 (s, 4H, Ar*-*m*-C*H*), 6.34 (s, 4H, Ar*-C*H*Ph$_2$), 5.92 (d, *J* = 2.2 Hz, 2H, XA-*p*-C*H*), 4.82 (d, *J* = 2.2 Hz, 2H, XA-*o*-C*H*), 2.89 (s, 12H, $^+$N(C*H*$_3$)$_4$), 2.10 (s, 6H, Ar*-C*H*$_3$), 1.57 (s, 6H, XA-C(C*H*$_3$)$_2$), 0.66 (s, 18H, XA-C(C*H*$_3$)$_3$) ppm.

^{13}C NMR (126 MHz, thf-d_8, 298 K) δ 153.3 (Ar*-*i*-*C*N), 149.5 (Ph-*i*-*C*), 148.6 (XA-*i*-*C*N), 145.4 (Ph-*i*-*C*), 144.5 (XA-*m*-*C*^{t}Bu), 143.0 (Ar*-*o*-*C*(CHPh$_2$)), 138.1 (XA-*o*-*C*O), 131.1 (Ph-*o*-*C*H), 131.1 (Ph-*o*-*C*H), 130.1 (Ar*-*m*-*C*H), 128.5 (Ar*-*p*-*C*), 128.4 (Ph-*m*-*C*H), 128.3 (Ph-*m*-*C*H), 127.9 (XA-*m*-*C*(C(CH$_3$)$_2$)), 125.9 (Ph-*p*-*C*H), 125.5 (Ph-*p*-*C*H), 109.8 (XA-*o*-*C*H), 104.1 (XA-*p*-*C*H), 55.8 ($^+$N(C*H*$_3$)$_4$), 52.2 (Ar*-*C*HPh$_2$), 34.9 (XA-*C*(CH$_3$)$_2$), 34.6 (XA-*C*(CH$_3$)$_3$), 33.6 (XA-*C*(CH$_3$)$_2$), 32.2 (XA-*C*(CH$_3$)$_3$), 21.8 (Ar*-*C*H$_3$) ppm.

Synthesis of [PPh_4][(^{Ar*}NON)CaCl(thf)] (4-PPh_4)

(^{Ar*}NON)Ca (12.4 mg, 0.01 mmol) and PPh_4Cl (3.7 mg, 0.01 mmol) and 0.5 mL thf-d_8 were added to a J. Young NMR tube. The solution was left at room temperature (or sonicated to speed up the reaction) until full conversion to **4**-PPh_4 was observed by ^{1}H NMR (2 h). The solution was then filtered and layered with an equal amount of hexane. Red crystals of **4**-PPh_4 formed over the course of 2 weeks, suitable for single crystal diffraction.

^{1}H NMR (400 MHz, thf-d_8, 298 K) δ 7.94 – 7.83 (m, 4H, $^+$$PPh_4$-*p*-C*H*), 7.78 – 7.64 (m, 16H, $^+$$PPh_4$-*o*-C*H,* $^+$$PPh_4$-*m*-C*H*), 7.23 – 7.14 (m, 8H, Ph-*o*-C*H*), 7.06 – 6.97 (m, 8H, Ph-*o*-C*H*), 6.91 – 6.76 (m, 20H, Ph-*m*-C*H,* Ph-*p*-C*H*), 6.71 (s, 4H, Ar*-*m*-C*H*), 6.75 – 6.65 (m, 4H, Ph-*p*-C*H*), 6.23 (s, 4H, Ar*-C*H*Ph_2), 5.88 (d, *J* = 2.2 Hz, 2H, XA-*p*-C*H*), 4.80 (d, *J* = 2.2 Hz, 2H, XA-*o*-C*H*), 2.00 (s, 6H, Ar*-CH_3), 1.55 (s, 6H, XA-C(CH_3)$_2$), 0.65 (s, 18H, XA-C(CH_3)$_3$) ppm.

^{31}P NMR (162 MHz, thf-d_8, 298 K) δ 23.0 ([*P*Ph_4]$^+$) ppm.

^{13}C NMR (126 MHz, thf-d_8, 298 K) δ 153.2 (Ar*-*i*-*C*N), 149.4 (Ph-*i*-*C*), 148.9 (XA-*i*-*C*N), 145.8 (Ph-*i*-*C*), 144.1 (XA-*m*-*C*^{t}Bu), 143.1 (Ar*-*o*-*C*($CHPh_2$)), 138.6 (XA-*o*-*C*O), 136.7 (d, *J* = 3.1 Hz, $^+$$PPh_4$-*p*-*C*H), 135.8 (d, *J* = 10.4 Hz, $^+$$PPh_4$-*m*-*C*H), 131.6 (d, *J* = 13.0 Hz, $^+$$PPh_4$-*o*-*C*H), 131.3 (Ph-*o*-*C*H), 131.2 (Ph-*o*-*C*H), 130.2 (Ar*-*m*-*C*H), 128.6 (Ar*-*p*-*C*), 128.2 (Ph-*m*-*C*H), 128.2 (Ph-*m*-*C*H), 128.1 (XA-*m*-*C*(C(CH_3)$_2$)), 125.6 (Ph-*p*-*C*H), 125.2 (Ph-*p*-*C*H), 119.2 (d, *J* = 89.5 Hz, $^+$$PPh_4$-*i*-*C*H), 109.5 (XA-*o*-*C*H), 103.2 (XA-*p*-*C*H), 52.3 (Ar*-*C*HPh_2), 35.0 (XA-*C*(CH_3)$_2$), 34.6 (XA-*C*(CH_3)$_3$), 33.2 (XA-*C*(CH_3)$_2$), 32.2 (XA-*C*(CH_3)$_3$), 21.9 (Ar*-*C*H_3) ppm.

Elemental analysis: anal. calc. for $C_{129}H_{134}CaClN_2O_5P$: C 81.59%, H 7.11%, N 1.48%, found: C 81.24%, H 6.85%, N 1.42%.

Synthesis of [K(2.2.2-crypt)][(^{Ar*}NON)CaF] (6-KCrypt)

(^{Ar*}NON)Ca (12.4 mg, 0.01 mmol), KF (1.2 mg, 0.02 mmol), 2.2.2-crypt (3.8 mg, 0.01 mmol), and 0.5 mL 2-MeThf were added to a J. Young NMR tube. The solution was subsequently heated at 80 °C until full conversion to [K(2.2.2-crypt)][(^{Ar*}NON)CaF] was observed (~12 days). The solution was then filtered and layered with an equal amount of hexane. Yellow crystals formed over the course of 6 days, suitable for single crystal diffraction.

^{19}F NMR (377 MHz, 2-MeThf, 298 K) δ -51.6 (Ca*F*) ppm.

Synthesis of [TMA]$_2$[(^{Ar*}NON)CaFCl] (7-TMA_2)

(^{Ar*}NON)Ca(thf) (9.8 mg, 7.5 µmol), TMACl (0.7 mg, 7.5 µmol), and 0.5 mL thf-d_8 were added to a J. Young NMR tube. The solution was subsequently heated at 80 °C until full conversion to [TMA][(^{Ar*}NON)CaCl(thf)] was observed. Then, TMAF (0.7 mg, 7.5 µmol) was added and left to equilibrate until no change in ratio of [TMA][(^{Ar*}NON)CaCl(thf)] and [TMA][(^{Ar*}NON)CaF(thf)] was seen (~3 days at RT, 1h at 80 °C). In solution, no species was detected that could be attributed to [TMA]$_2$[(^{Ar*}NON)CaFCl] (hence, no NMR data can be provided for this compound). Crystals suitable for single crystal Xray diffraction were grown by slow evaporation of the filtered solution.

Synthesis of biphenyl-4-d_2-methanol

Biphenyl-4-carboxylic acid (1.0 g, 5.0 mmol) was added to a Schlenk flask containing a stirrer bar and placed under argon atmosphere by 3 vacuum-argon cycles. After anhydrous Et_2O (25 ml) was added and the mixture was cooled to 0 °C, $LiAlD_4$ (0.63 g, 15 mmol) was added slowly in 3 portions under a light flow of Argon and strong stirring. After the additions, the suspension was allowed to warm up by removing the ice bath and stirred for 2h at room temperature. The reaction was quenched with H_2O and 1M HCl (until solid has dissolved; ~20 and 20 ml, respectively) and extracted with Et_2O (3x25 ml). The combined organic extracts were then washed with brine (25 ml), dried with $MgSO_4$, and evaporated to dryness to yield biphenyl-4-d_2-methanol in quantitative yield (0.93 g).

^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ 7.63 – 7.56 (m, 4H), 7.47 – 7.41 (m, 4H), 7.35 (t, *J* = 7.4 Hz, 1H), 4.73 (s, <1% $d_{<2}$-product), 1.63 (s, 1H) ppm.

^{2}D NMR (77 MHz, $CDCl_3$, 298 K) δ 4.73 (s, 2D) ppm.

Spectroscopic data are in accordance with those in literature (^{1}H NMR).[6,7]

Synthesis of 4-(bromo-d_2-methyl)-biphenyl

Biphenyl-4-d_2-methanol (0.93 g, 5.0 mmol) and Et_2O (8 ml) were added to a round bottom flask with stirrer bar. After CBr_4 (1.82 g, 5.5 mmol) and PPh_3 (1.44 g, 5.5 mmol) were added, the mixture was stirred for 2h at room temperature. The reaction mixture was evaporated to dryness, redissolved in DCM and loaded onto celite for purification by flash column chromatography (3% Et_2O in cyclohexane) to result in 78% 4-(bromo-d_2-methyl)-biphenyl (0.96 g).

^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ 7.61 – 7.55 (m, 4H, Ph_{sub}-*o*-C*H*, Ph_{uns}-*o*-C*H*), 7.50 – 7.43 (m, 4H, Ph_{sub}-*m*-C*H*, Ph_{uns}-*m*-C*H*), 7.37 (t, *J* = 7.4 Hz, 1H, Ph_{uns}-*p*-C*H*), 4.55 (s, <1% $d_{<2}$-product for -CD_2Br) ppm.

^{2}D NMR (77 MHz, $CDCl_3$, 298 K) δ 4.54 (s, 2D, -CD_2Br) ppm.

^{13}C NMR (126 MHz, $CDCl_3$, 298 K) δ 141.5 (Ph_{sub}-*i*-*C*H), 140.6 (Ph_{uns}-*i*-*C*H), 136.8 (Ph_{sub}-*p*-*C*), 129.6 (Ph_{sub}-*m*-*C*H), 129.0 (Ph_{uns}-*m*-*C*H), 127.7 (Ph_{uns}-*p*-*C*H), 127.7 (Ph_{sub}-*o*-*C*H), 127.3 (Ph_{uns}-*o*-*C*H), 33.1 (p, *J* = 23.6 Hz, -*C*D_2Br) ppm.

Spectroscopic data are in accordance with those in literature (^{1}H NMR).[6,7]

2. Supplementary data

Isolation of terminal calcium fluoride complexes

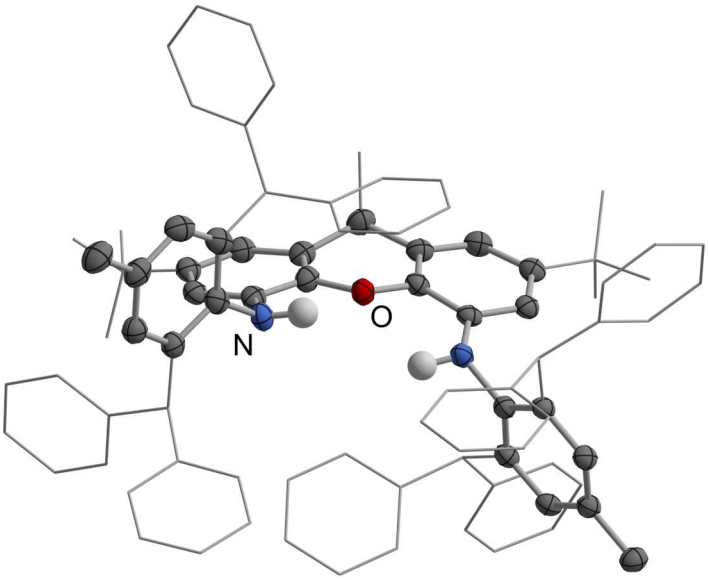


***Figure S 1**. Molecular structure of $^{Ar*}NONH_2$ in the solid state, as determined by X-ray crystallography. Thermal ellipsoids set at the 50% level. Selected hydrogen atoms, solvate molecule and second disorder component omitted, and selected fragments shown in wireframe format for clarity.*

Supplementary discussion 1

Attempted syntheses of ^{Ar*}NONCa(thf)$_x$ from Ca{N(SiMe$_3$)$_2$}$_2$(thf)$_2$ and ^{Ar*}NONH$_2$ in benzene did not yield any product (in contrast to the sterically less demanding Dipp and Trip analogues). Instead, a two-step process was required comprised of ^{Ar*}NONH$_2$ deprotonation with KH to form K$_2$[^{Ar*}NON] (Fig. S2), followed by the reaction with CaI$_2$ in thf. Depending on the coordinating ability of the solvent used in the final step of the work up of (^{Ar*}NON)Ca(thf)$_x$ (i.e. thf or toluene) the NMR signals for thf would either be present or absent, respectively (without any heating of the complex under vacuum). Crystallization of these complexes confirmed that the thf-free complex (^{Ar*}NON)Ca (**1**, x = 0), as well as the mono- (x = 1) and bis-thf (x = 2) derivatives (**1**-thf and **1**-thf$_2$, resp.) can readily be obtained from the same reaction mixture by minor modification of the work-up protocol (Fig. S3). A solvent free (^{XXX}NON)Ca complex to the best of our knowledge has not yet been reported, although a bis-arene complex (^{Dipp}NON)Ca(C$_6$H$_6$)$_2$ has been reported by Hicks and co-workers to be formed from the corresponding bis(diethyl ether) system (requiring heating to 150 °C under high vacuum of 1 × 10^{-2} mbar)[8].

The isolation of the three complexes speaks to a degree of flexibility in the ^{Ar*}NON ligand scaffold which allows small molecules/ions to access the metal coordination site on rotation of its flanking phenyl groups. The solid-state structure of (^{Ar*}NON)Ca(thf)$_2$ is comparable to that of (^{Dipp}NON)Ca(thf)$_2$ with a geometry in between of square pyramidal (SP) and trigonal bipyramidal (TBP) (τ = 0.62 and 0.66, respectively). A phenyl ring on the bottom face provides some degree of steric protection but is still far from coordinating to the Ca (Ca–Ph$_{centroid}$ distance: 4.724(1) Å). (^{Ar*}NON)Ca(thf) can be regarded as a derivative in which the apical thf replaced by a flanking phenyl group (Ca– Ph$_{centroid}$ distance: 2.927(1) Å). Additionally, the bottom phenyl group approaches the Ca center further with a Ca– Ph$_{centroid}$ distance of 4.161(1) Å. Alternatively, the complex can be described with a distorted square planar geometry around the calcium centre (sum of angles: 350.5(1)°) when disregarding the phenyl substituents.

The isolation of a solvent-free (^{Ar*}NON)Ca system (**1**-□) demonstrates the enhanced steric demands of the (^{Ar*}NON) ligand scaffold, and its potential for intra-molecular arene coordination (Fig. 2G). **1**-□ can be described as a distorted T-shape (N–Ca–O–N torsion angle of 0.6(1)°) or, when accounting for close contacts with the phenyl groups of the diphenylmethyl substituents (Ca–Ph$_{centroid}$ distances: 2.733(1) and 2.825(2) Å), as a distorted trigonal bipyramid in which the oxygen atom and the two phenyl centroids form a near perfect basal plane (inter-ligand angles of 114.7(1)°, 122.5(1)°, and 122.8(1)° with a torsion angle of <1°). The amide nitrogens then constitute (somewhat distorted) axial substituents (N–Ca–N 136.0(1)°). Noteworthily, the Ca–Ph$_{centroid}$ interactions effectively shroud the calcium center from the top and bottom faces and from end-on approach (in contrast to the steric profile offered by the ^{Trip}NON/^{Dipp}NON scaffolds).

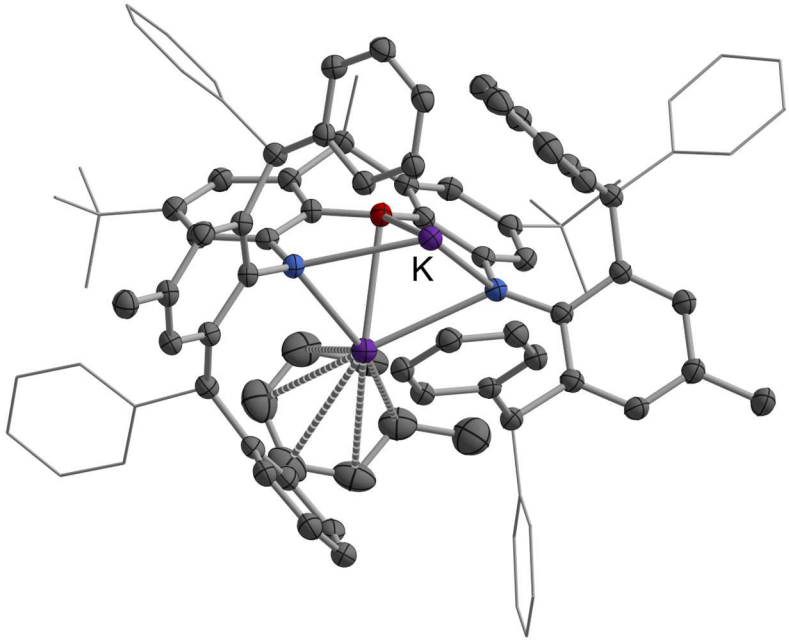


***Figure S 2**. Molecular structure of $^{Ar*}NONK_2$ in the solid state, as determined by X-ray crystallography. Thermal ellipsoids set at the 50% level. Hydrogen atoms omitted and selected fragments shown in wireframe format for clarity.*

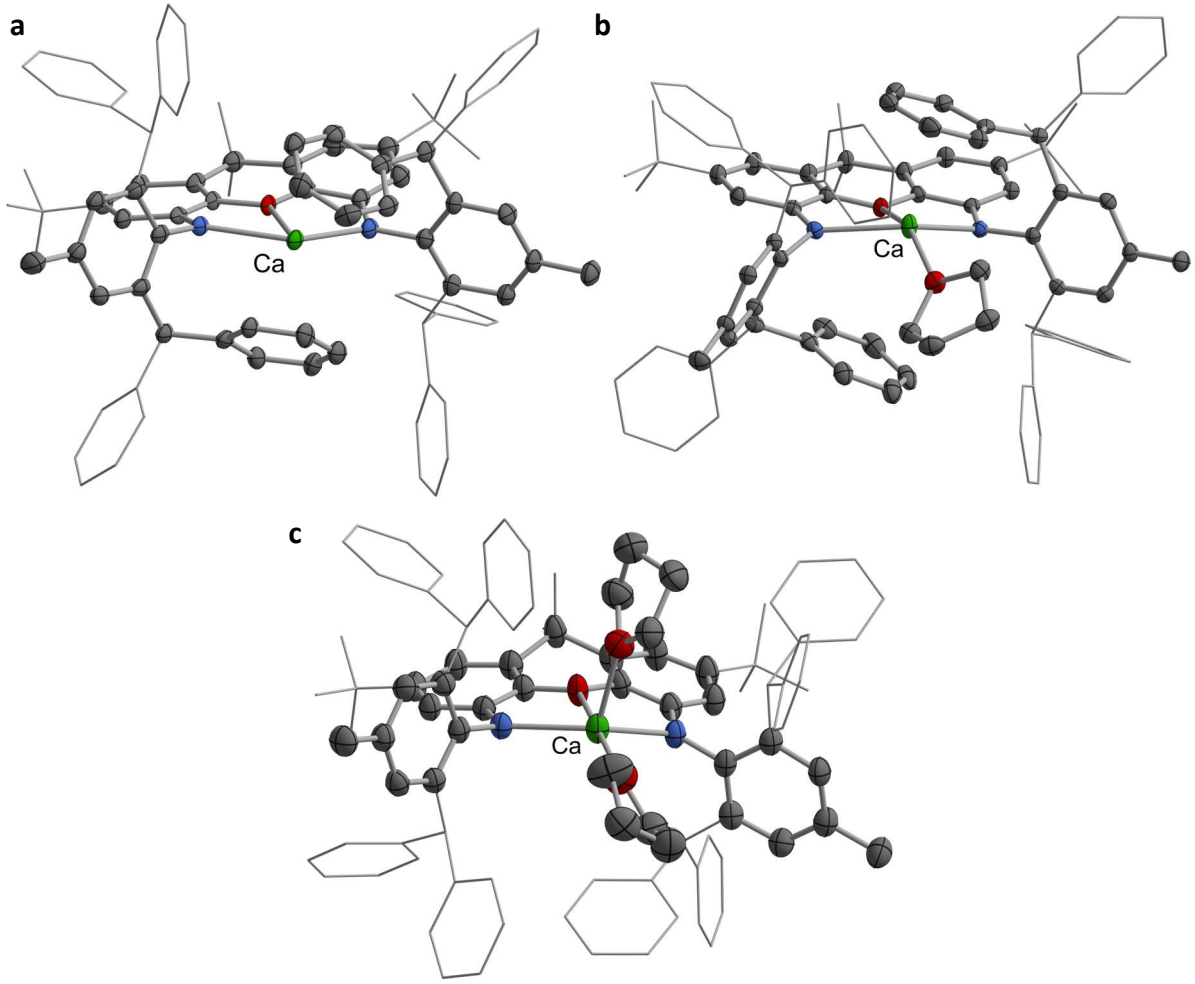


Figure S 3. *Molecular structures of (^{Ar*}NON)Ca (**1**-□, a), (^{Ar*}NON)Ca(thf) (**1**-thf, b), and (^{Ar*}NON)Ca(thf)$_2$ (**1**-thf$_2$, c) in the solid state, as determined by X-ray crystallography. Thermal ellipsoids set at the 50% level. Hydrogen atoms, solvate molecules and second disorder components omitted, and selected fragments shown in wireframe format for clarity. The structure of (^{Ar*}NON)Ca(thf)$_2$ was collected at 200 K, as a destructive phase transition occurred at lower temperatures.*

Supplementary discussion 2

To confirm the identities of species observed by ^{19}F NMR at δ_F = –55.8 ppm and –72.9 ppm, we carried out X-ray crystallographic studies. Crystallization from a reaction mixture containing two equivalents of fluoride confirms that the species at –72.9 ppm is a monomeric calcium-difluoride complex featuring two $[NMe_4]^+$ counterions, i.e. $[NMe_4]_2[(^{Ar^*}NON)CaF_2]$ (**3**-TMA_2, Fig 2C). Interestingly however, all attempts to crystallize from a 1:1 reaction mixture also generate crystals of **3**-TMA_2, with the supernatant solution in this case showing the formation of fluoride-free **1**. Moreover, redissolving crystals of **3**-TMA_2 in the supernatant was found to re-establish the equilibrium favouring monofluoride **2**-TMA, and the addition of one equivalent of **1** to a solution of **3**-TMA_2 leads to quantitative generation of **2**-TMA (as judged by ^{19}F NMR, Fig. 2A-B). Thus, although in solution the equilibrium established between **1** and TMAF (in a 1:1 ratio) lies on the side of monofluoride **2**-TMA, this equilibrium is not reflected by the solid-state product, presumably reflecting the lower solubility/greater crystallinity of the divalent $[NMe_4]_2[(^{Ar^*}NON)CaF_2]$ salt.

To further investigate the generality of the phenomenon in which the equilibrium in solution is not reflected by the obtained solid-state product, the analogous reaction with $[NMe_4]Cl$ (TMACl) was performed (Fig. 2D). Reacting one equivalent of TMACl with **1** proceeds cleanly to one product, attributed to the monochloride complex (**4**-TMA) as confirmed by integration of the anion/cation signals in the ^1H NMR spectrum. In this case, however, the addition of a second equivalent of TMACl did not result in the formation of a new species, with the signals due to **4**-TMA remaining unchanged, alongside solid TMACl. Despite the lack of any evidence for the formation of a calcium dichloride adduct in solution, however, crystallization from thf solutions resulted exclusively in the isolation of $[TMA]_2[(^{Ar^*}NON)CaCl_2]$ (**5**-TMA_2, Figure S4). Similarly, although the addition of TMAF to **4**-TMA in thf leads to a mixture of mono-fluoro and mono-chloro species in solution (as evidenced by ^1H and ^{19}F NMR spectroscopy matching **2**-TMA and **4**-TMA), crystallization resulted in the mixed halide $[TMA]_2[(^{Ar^*}NON)Ca(F)Cl]$ (**7**-TMA_2, Figure S4). These examples therefore form a consistent picture in which the solution equilibria and solid-state products are mismatched in a reversible manner.

Reasoning that the differences between solution and solid-state behaviour might reflect the free-energy associated with crystal packing, we targeted fluoride sources with large rigid counter-cations such as $[PPh_4]^+$ that could favour the crystallization of the monofluoride[9,10]. The 1:1 reaction of $[PPh_4]F$ with **1** in thf immediately and quantitatively generates one species, as judged by ^1H and ^{19}F NMR spectroscopy, which was shown to be $[PPh_4][(^{Ar^*}NON)CaF(thf)]$ (**2**-PPh_4) both in solution and the solid-state (Fig. 2E-F). The crystal structure features a monomeric calcium-fluoride complex containing an axial (terminal) fluoride ligand, with a thf molecule occupying the equatorial position. In a similar fashion, $[PPh_4][(^{Ar^*}NON)CaCl(thf)]$ (**4**-PPh_4, Fig. S5) is formed in the reaction of **1** with $[PPh_4]Cl$ in thf. Addition of a second equivalent of $[PPh_4]F$ to a thf-solution of **2**-PPh_4 results in the formation of the difluoride complex $[PPh_4]_2[(^{Ar^*}NON)CaF_2]$ (**3**-$(PPh_4)_2$, δ_F=−71.3 ppm), which has a solid-state structure very similar to TMA-**3** (Fig. S6).

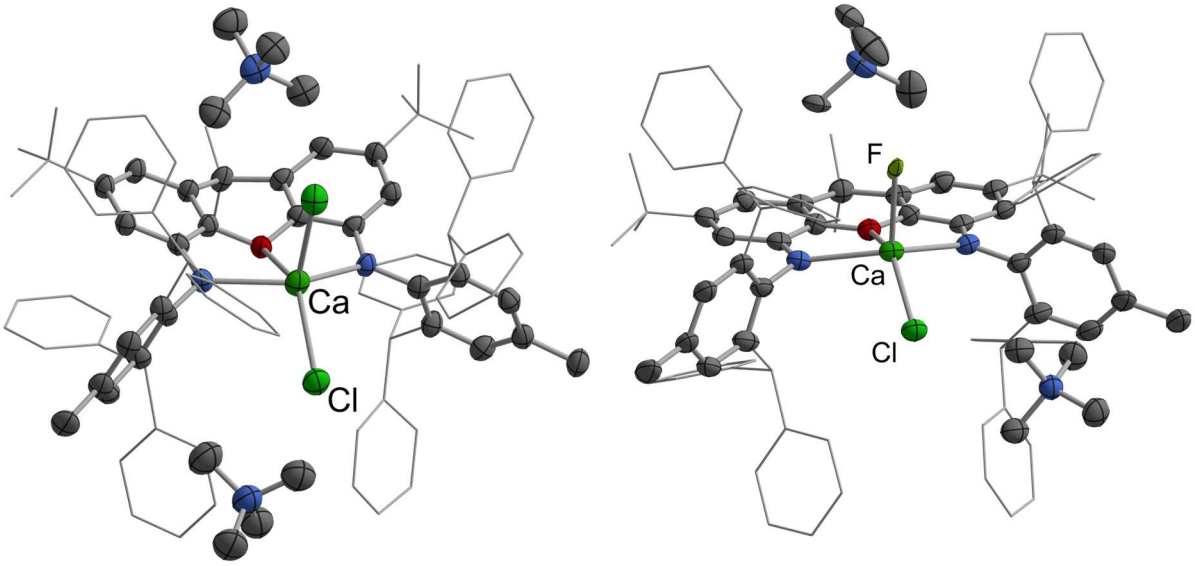


***Figure S 4**. Molecular structures of [TMA]$_2$[^{Ar*}NONCaCl$_2$] (**5**-TMA$_2$, left) and [TMA]$_2$[^{Ar*}NONCaFCl] (**7**-TMA$_2$, right) in the solid state, as determined by X-ray crystallography. Thermal ellipsoids set at the 50% level. Hydrogen atoms, solvate molecules and second disorder component omitted, and selected fragments shown in wireframe format for clarity.*

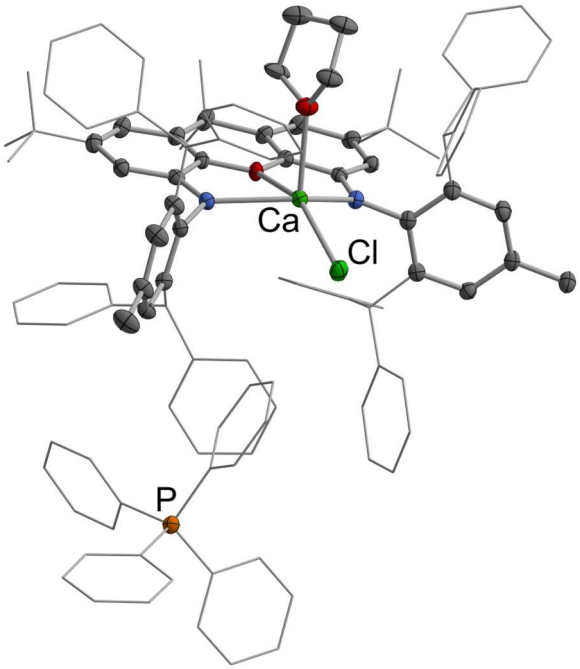


***Figure S 5**. Molecular structure of the monochloride [PPh$_4$][^{Ar*}NONCaCl(thf)] (**4**-PPh$_4$) in the solid state, as determined by X-ray crystallography. Thermal ellipsoids set at the 50% level. Hydrogen atoms, solvate molecules and second disorder component omitted, and selected fragments shown in wireframe format for clarity. Compared to **2**-PPh$_4$ the positions of the halide and thf ligands at calcium in the solid-state are switched (presumably on steric grounds).*

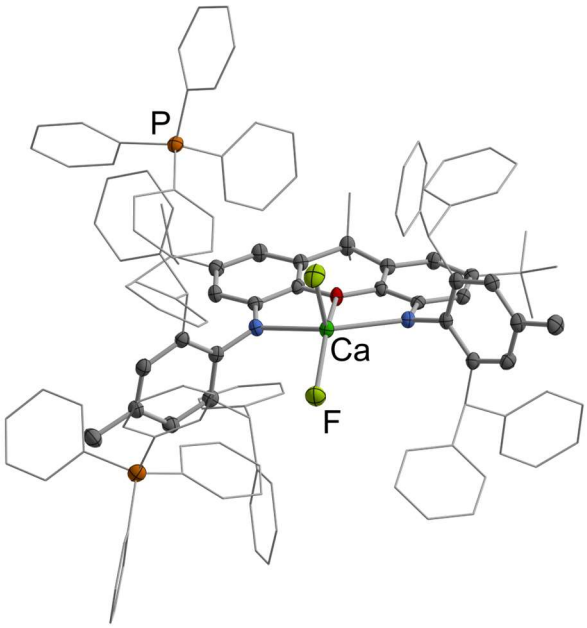


***Figure S 6**. Molecular structures of the difluoride $[PPh_4]_2[^{Ar^*}NONCaF_2]$ (**3**-$(PPh_4)_2$) in the solid state, as determined by X-ray crystallography. Thermal ellipsoids set at the 50% level. Hydrogen atoms, solvate molecules and second disorder component omitted, and selected fragments shown in wireframe format for clarity.*

Supplementary discussion 3

The generation of calcium-fluoride complexes from **1** and potassium fluoride directly was also investigated. The reactions of **1** with KF lead to no conversion either in benzene or thf solution, even in the presence of 18-crown-6 (or its mono- or dibenzo derivatives). Refluxing **1** with KF in thf in the presence of the more potent sequestering agent 2.2.2-cryptand, on the other hand, leads to the selective formation of a single species over 4 days, giving rise to a ^{19}F NMR signal at δ_F = −53.4 ppm. In the solid state, both the mono- and difluoride were obtained upon layering thf solutions with hexane, reminiscent of the solution/solid-state mismatch observed earlier. A low-quality X-ray structure of [K(2.2.2-crypt)][(^{Ar*}NON)CaF(thf)] (**2**-KCrypt) could be obtained (Fig. S7) confirming connectivity and revealing the presence of an axial fluoride ligand with a molecule of thf in the equatorial position (as per **2**-PPh_4). The generation of the thf-free analogue of **2**-PPh_4 also proceeds readily in 2-MeThf, however no crystals were obtained suitable for single-crystal diffraction.

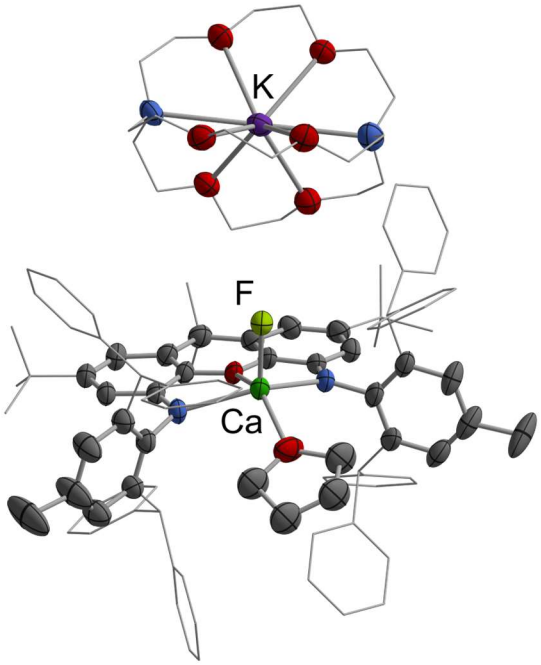


***Figure S 7**. Molecular structure of [K(2.2.2-crypt)][^{Ar*}NONCaF(thf)] (**2**-KCrypt) in the solid state, as determined by X-ray crystallography. Thermal ellipsoids set at the 30% level. Hydrogen atoms, solvate molecules and second disorder component omitted, and selected fragments shown in wireframe format for clarity. Structure displayed for connectivity purposes only.*

Reactivity of terminal calcium fluorides

Supplementary discussion 4

The reaction of **2**-PPh_4 with 1-adamantylcarbonyl chloride (AdCOCl) at room temperature proceeds quantitatively and in <5 min to the product AdCOF (Fig. 4A, left). The calcium complex itself is converted cleanly to one product with its ^{1}H NMR spectrum matching the independently synthesized chloride complex **4**-PPh_4. Also for electrophiles with other leaving groups (e.g. bromide or azide), the resulting calcium center features the respective leaving group. Analogously, both fluorides from the CaF_2 fragment in **3**-TMA are delivered quantitatively to AdCOCl in <5 min (Fig. 4A right). Addition of AdCOCl to a solution of **3**-TMA_2 resulted in the immediate formation of a quantitative yield of AdCOF and a white precipitate (in contrast to the monofluoride). From the mass balance of the reaction together with the observation that chloride complex **4**-TMA is the sole Ca-containing product observed by ^{1}H NMR, it can be concluded that $[Me_4N]Cl$ precipitates from the reaction. It is hypothesized that the mixed halide complex $[(^{Ar*}NON)Ca(F)Cl]^{2-}$ is formed transiently after via fluoride/chloride exchange with the substrate, which rapidly dissociates in solution into $[(^{Ar*}NON)Ca(thf)F]^-$ and $[Me_4N]Cl$ according to the behaviour established previously. The delivery of a second fluoride equivalent from $[(^{Ar*}NON)Ca(thf)F]^-$ then follows the same mechanism as the mono-fluoride complex.

General procedure

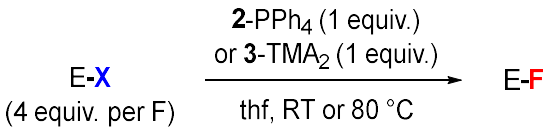


Figure S 8 *Reaction scheme for fluoride transfer from* ***2****-PPh_4 or* ***3****-TMA_2 (0.005 mmol complex, 1 equiv.) to C(sp^2), C(sp^3), S, Si, and P based electrophiles (i.e., AdCOCl, 1-bromopentane, Ph_3CBr, TsCl, Ph_3SiCl, Ph_3SiN_3, PPh_3Cl_2; 4 equiv.). All reactions were performed in a J-Young NMR tube at room temperature (except for reactions with 1-bromopentane at 80 °C where indicated). All products matched characterization reported in literature[11–15]. All yields were determined by quantitative ^{19}F NMR spectroscopy with PhF (5 µL) as internal standard (the integrated standard was set to 100 and the yield subsequently calculated from the product integral and the starting material integral before reaction). Attempted reactions with 2,4-dinitrochlorobenzene and 1-iodoadamantane did not lead to any product formation. Selected examples are given in* ***Figure S 9****-****Figure S 17****.*

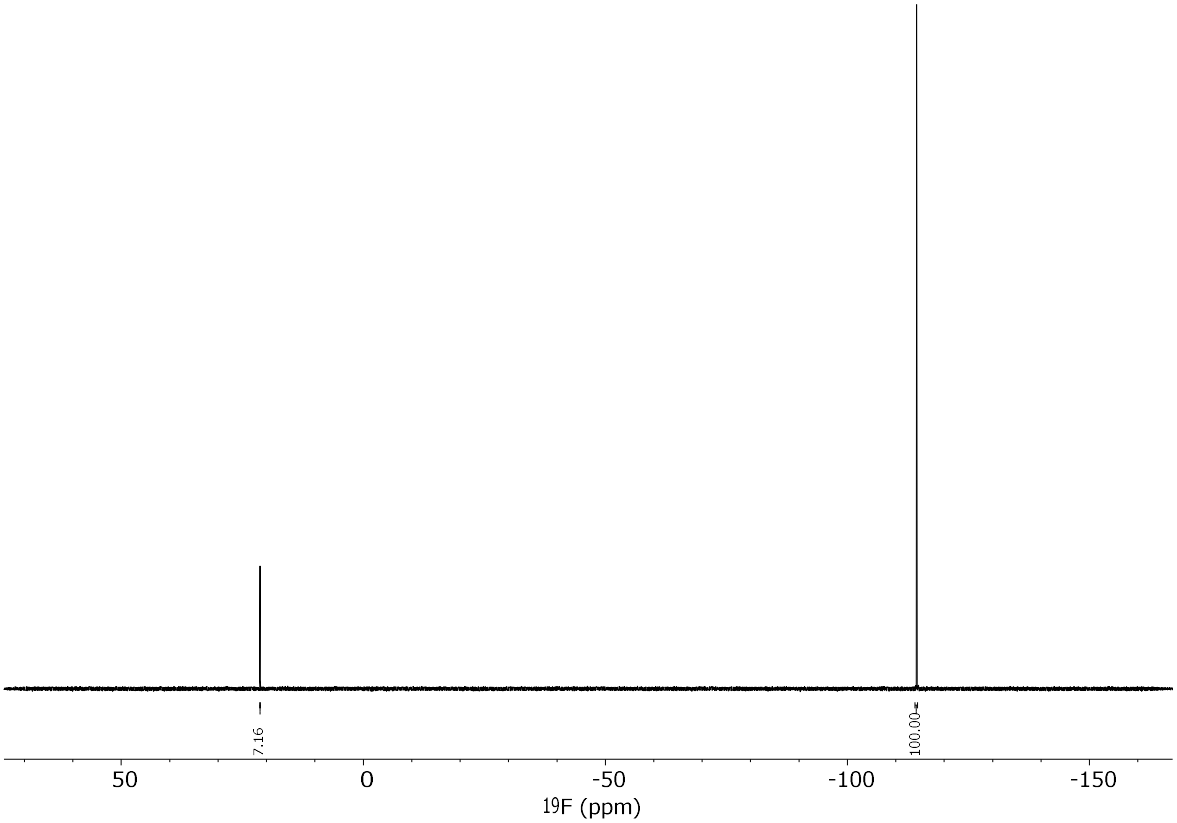


Figure S 9 *Quantitative ^{19}F NMR spectrum for the reaction of **2**-PPh_4 with AdCOCl in thf after 5 min at RT. Starting material integral before reaction: 7.16.*

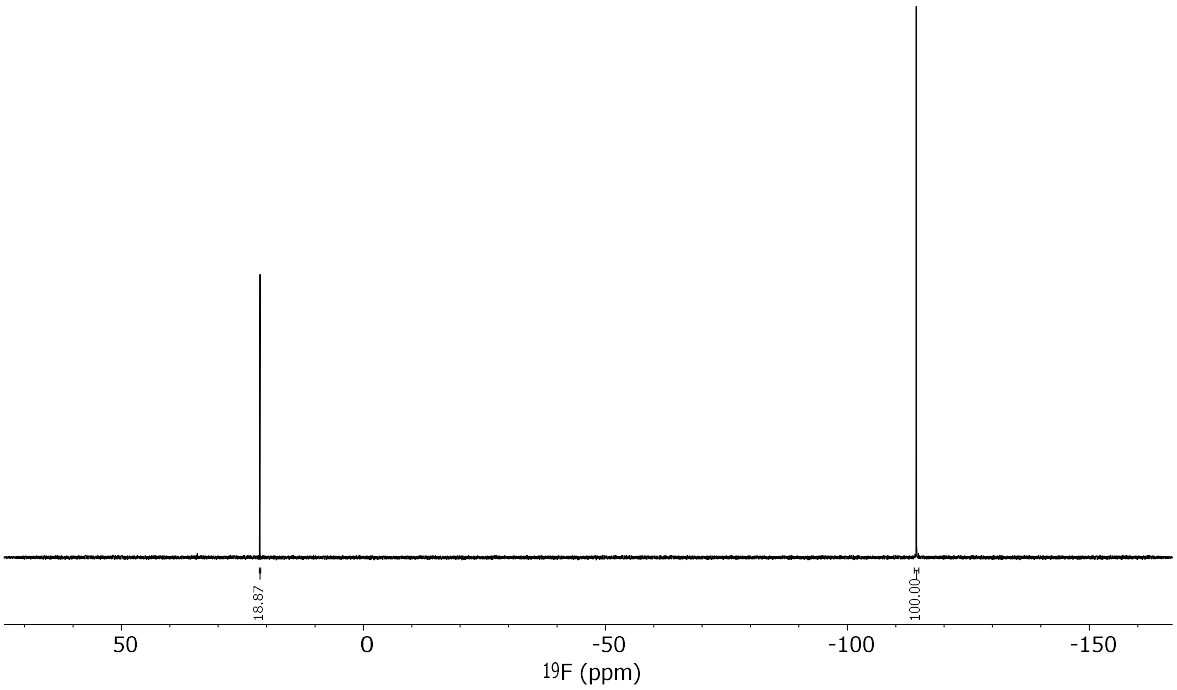


Figure S 10 *Quantitative ^{19}F NMR spectrum for the reaction of **3**-TMA_2 with AdCOCl in thf after 5 min at RT. Starting material integral before reaction: 18.86.*

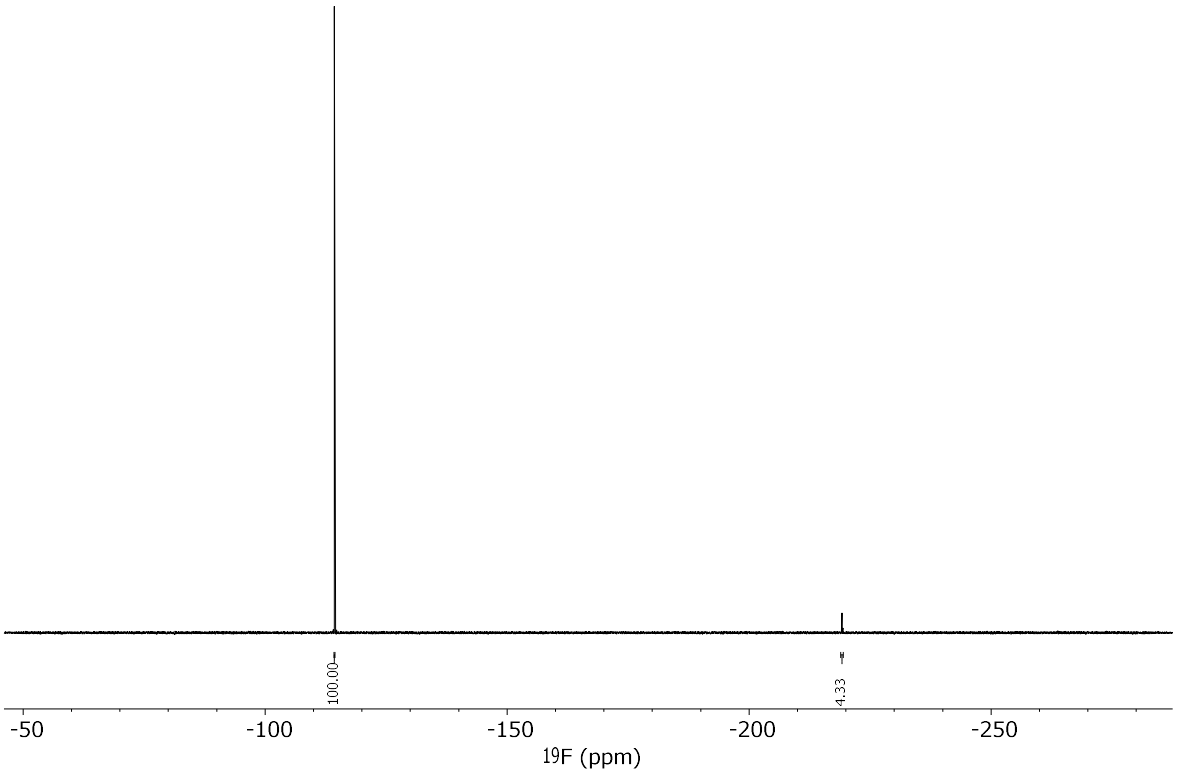


Figure S 11 *Quantitative ^{19}F NMR spectrum for the reaction of **2**-PPh_4 with 1-bromopentane in thf after 72 h at 80 °C. Starting material integral before reaction: 7.20.*

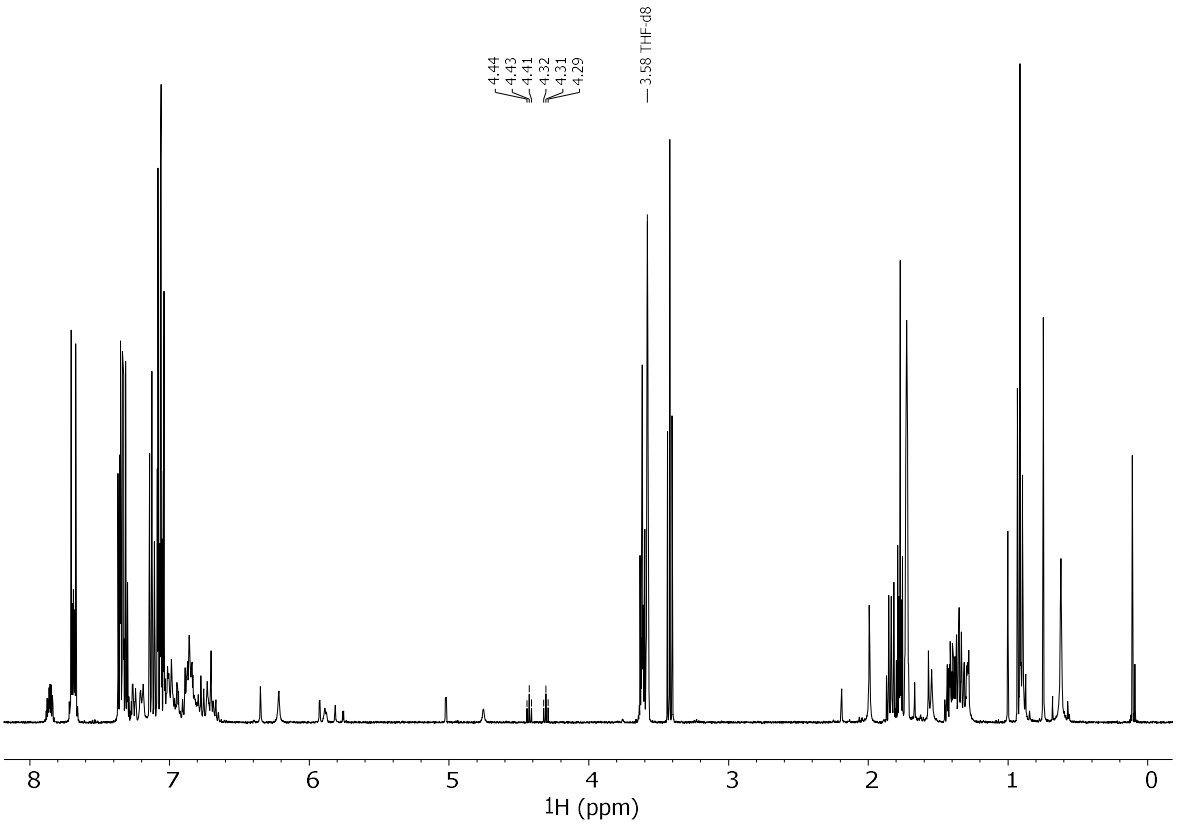


Figure S 12 *^{1}H NMR spectrum for the reaction of **2**-PPh_4 with 1-bromopentane in thf demonstrating the formation of 1-fluoropentane and the absence of 1-pentene.*

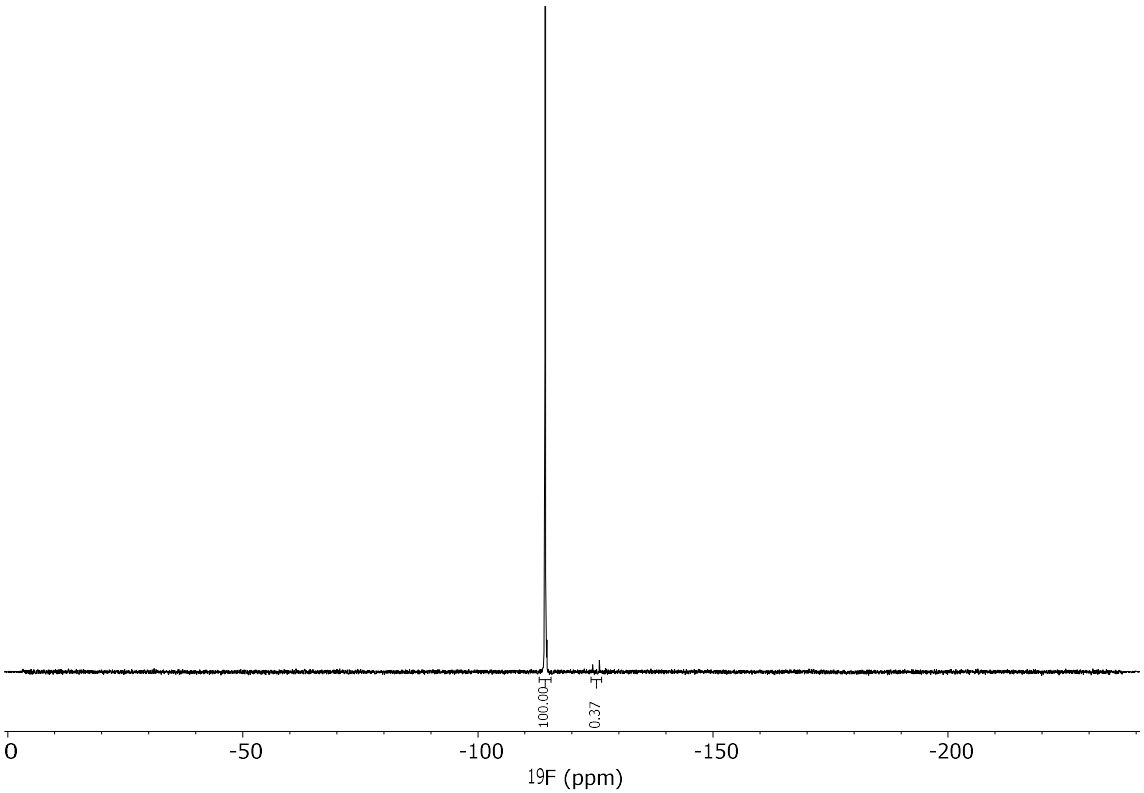


Figure S 13 *Quantitative ^{19}F NMR spectrum for the reaction of **2**-PPh_4 with Ph_3CBr in thf immediately after addition (<2 min) at RT. Starting material integral before reaction: 7.27. The product Ph_3CF was found to degrade quickly after its formation under the reaction conditions and thus no reliable yield determination of the can be made.*

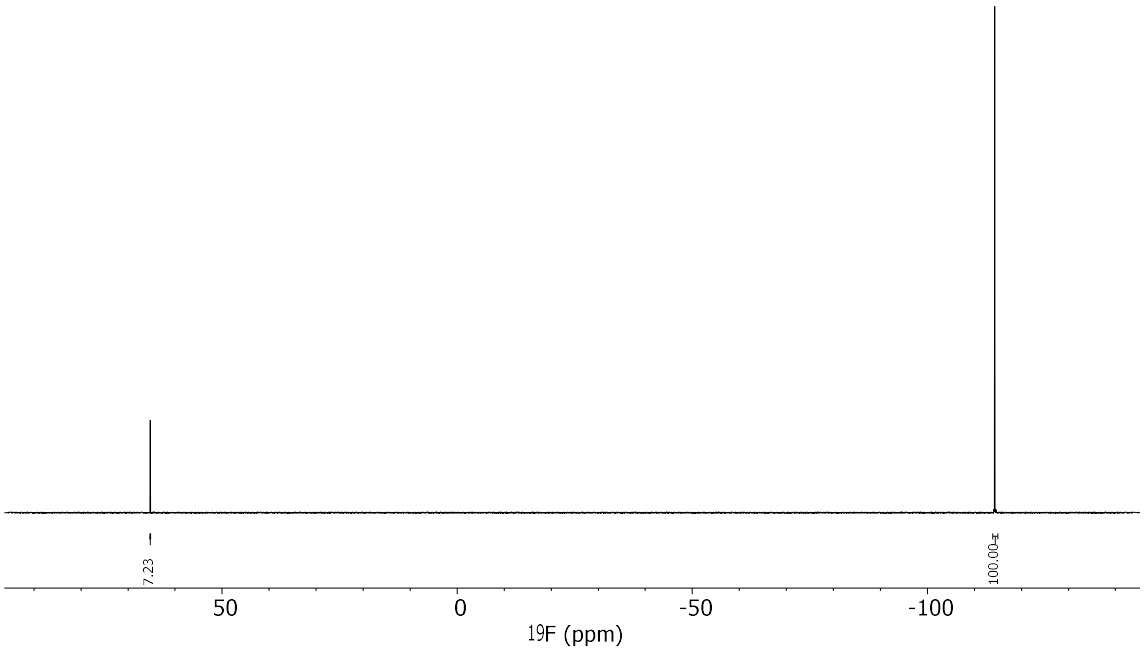


Figure S 14 *Quantitative ^{19}F NMR spectrum for the reaction of **2**-PPh_4 with TsCl in thf after <15 min at RT. Starting material integral before reaction: 7.21.*

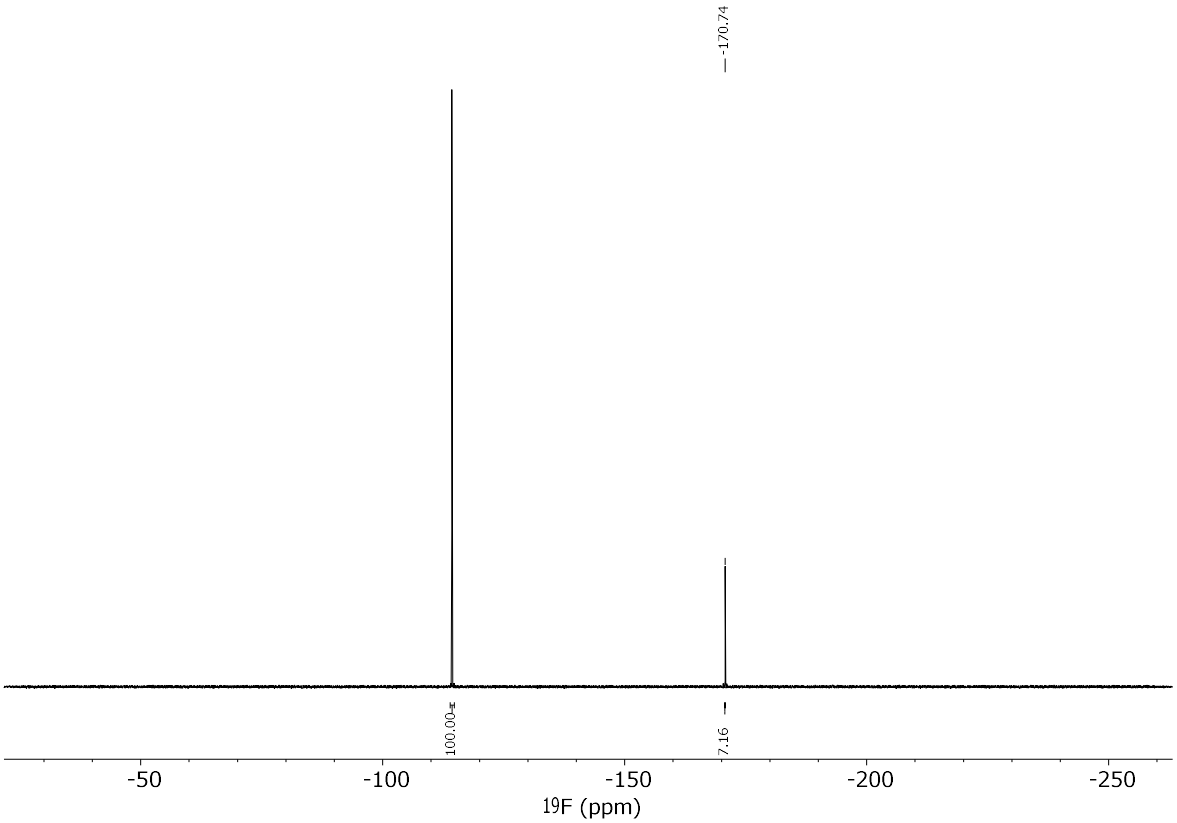


Figure S 15 *Quantitative ^{19}F NMR spectrum for the reaction of **2**-PPh_4 with Ph_3SiCl in thf after <15 min at RT. Starting material integral before reaction: 7.17.*

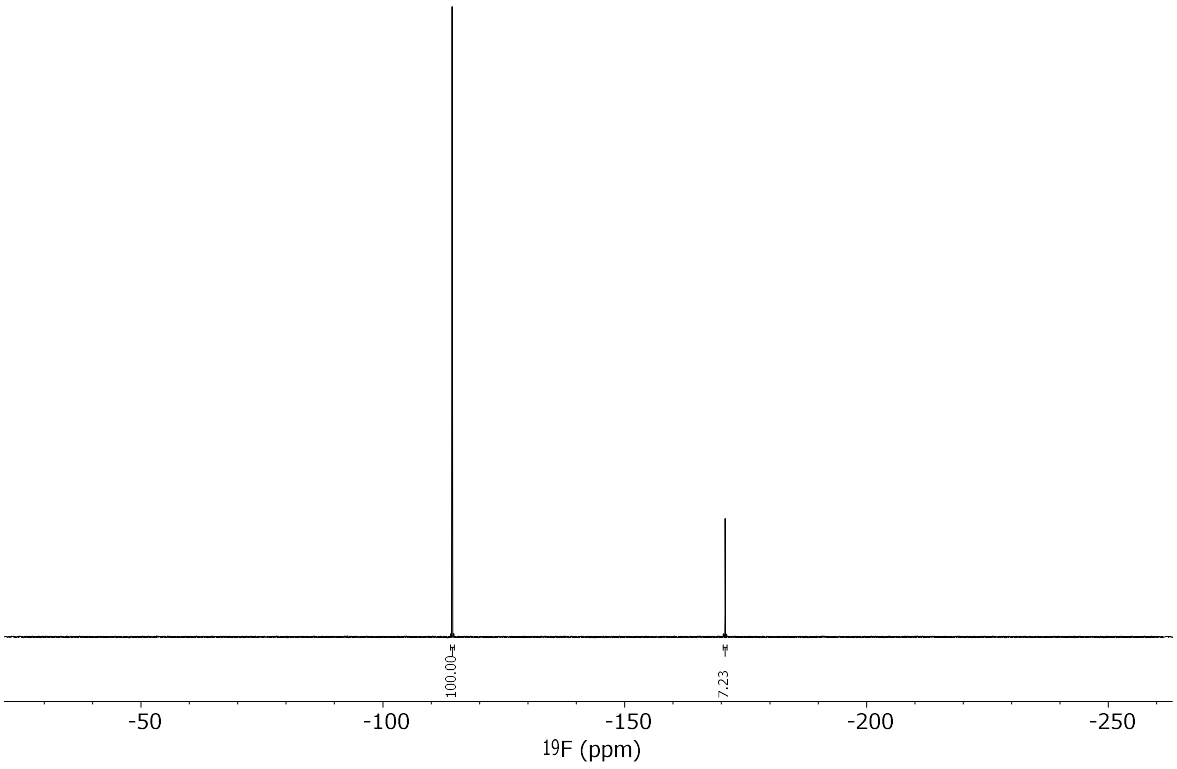


Figure S 16 *Quantitative ^{19}F NMR spectrum for the reaction of **2**-PPh_4 with Ph_3SiN_3 in thf after <15 min at RT. Starting material integral before reaction: 7.22.*

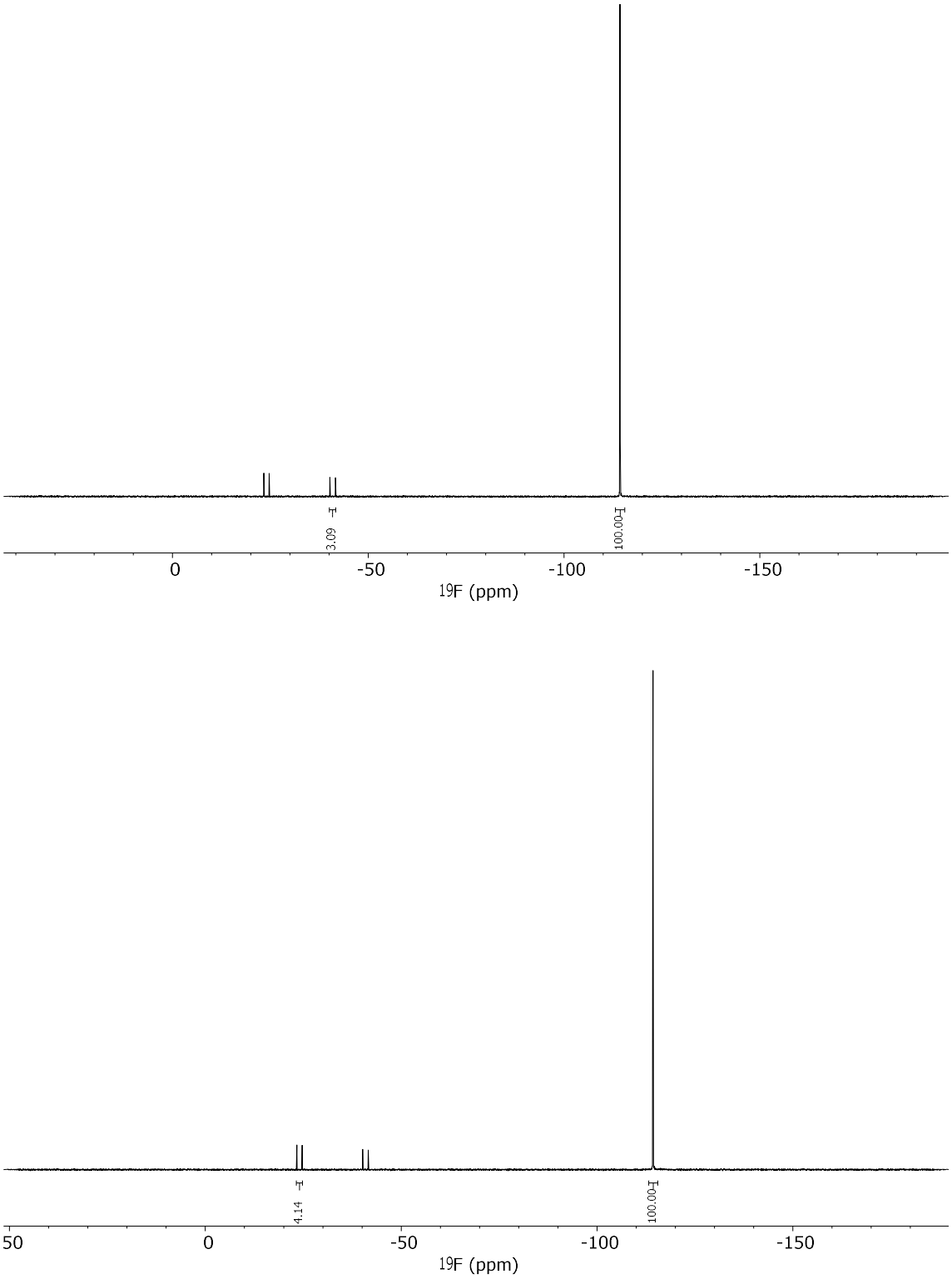


Figure S 17 *Quantitative ^{19}F NMR spectrum for the reaction of* ***2****-PPh_4 with PPh_3Cl_2 in thf after <15 min at RT. For the yield the total amount of F in P-F bonds from a mixture of PPh_3F_2 (at -40.9 ppm) and monofluorinated product (at -24.0 ppm) was used. To obtain the most reliable results (i.e., ensure that the centre of the spectrum is between the internal standard and the product peak), two spectra were acquired with different midpoints. Starting material integral before reaction: 7.21.*

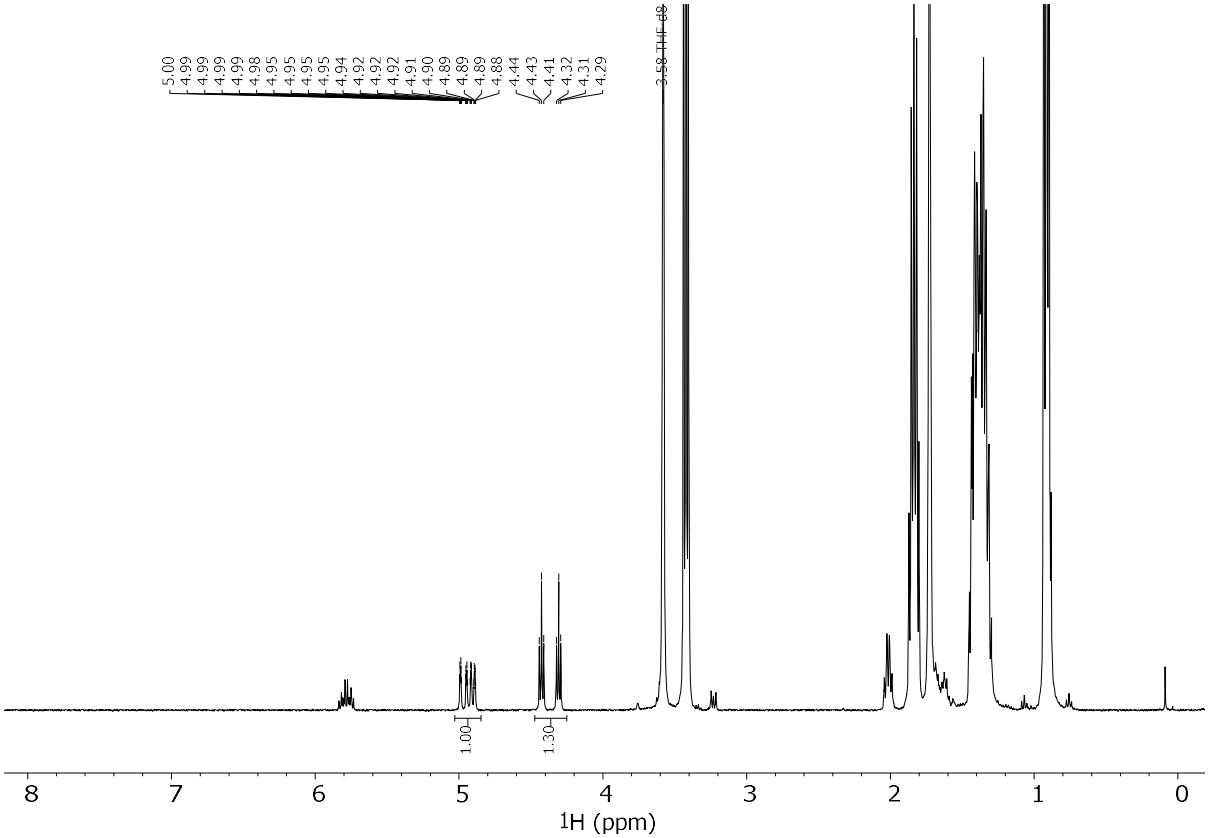


Figure S 18 *Quantitative ^{1}H NMR spectrum for the reaction of 1-bromopentane with TMAF in thf at room temperature after 5 days. A ratio of ~1:1.3 1-pentene:1-fluoropentane is formed.*

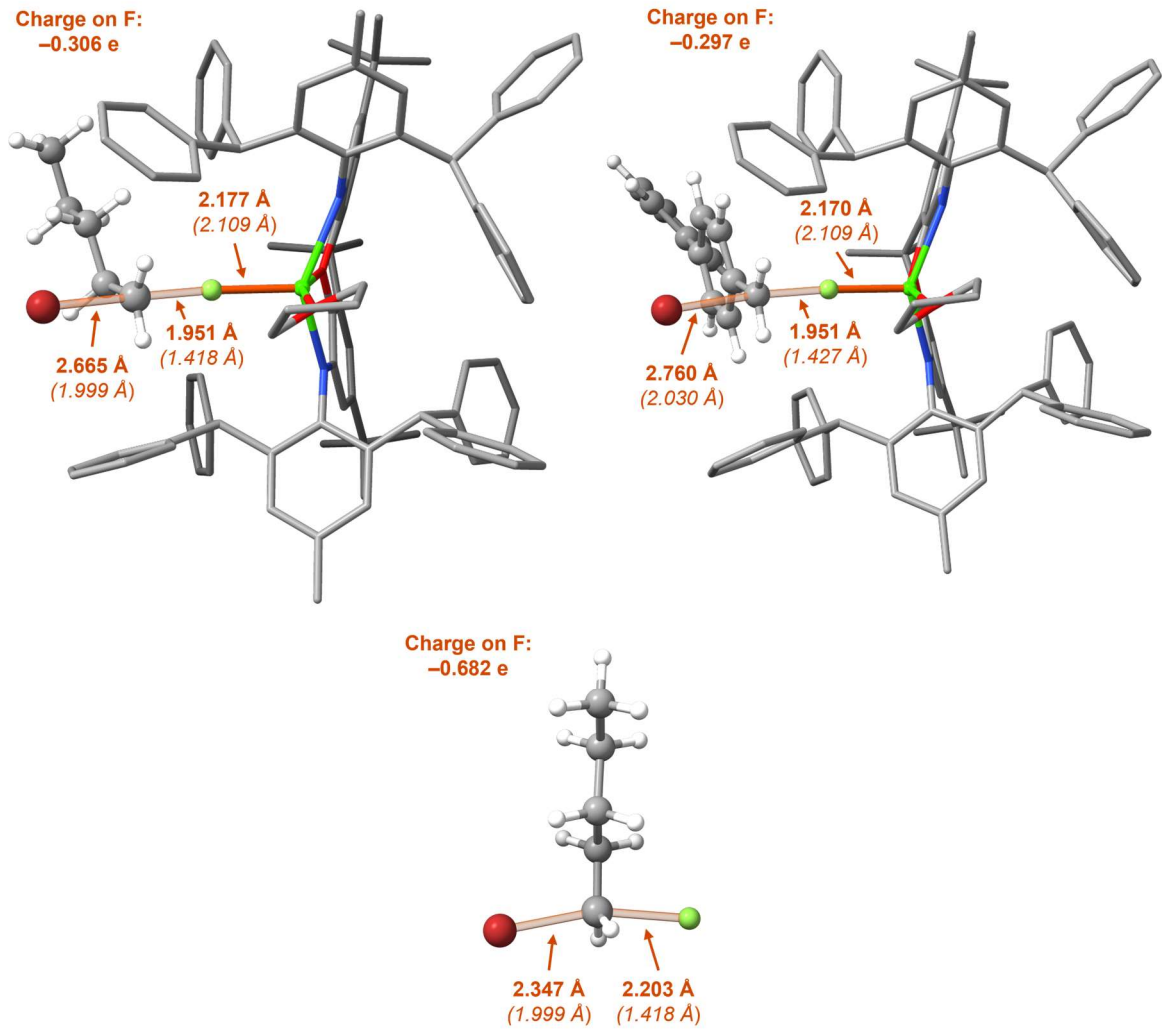


Figure S 19 *Transition state for Ca-F retention (TS1a, Fig 3) during fluoride delivery to 1-bromopentane (top left) and 4-(bromomethyl) biphenyl (top right), versus full Ca-F dissociation (TS1b, Fig 3) during fluoride delivery to 1-bromopentane (bottom). Bond lengths in the transition-state are given in bold with their length in the respective free molecule as reference. (R–Br, R–F, and* ***2****-PPh_4 for C–Br, C–F, and Ca–F, respectively). VDD charge on the fluoride at the transition state is given top left. For fluorination by* ***2****-PPh_4 (top), the Ca–F bond remains nearly unaltered (Δd = 0.068 and 0.061 Å) in the transition-state where the C–F is already closer to being formed (Δd = 0.533 and 0.524 Å) and the C–Br is already more broken in the transition-state (Δd = 0.666 and 0.730 Å, respectively). Moreover, the VDD charges on the fluoride are lower compared to the case for full Ca-F pre-dissociation (bottom).*

Calcium-catalyzed fluorination using KF

Summary of initial experiments into the performance of other group 2 metals

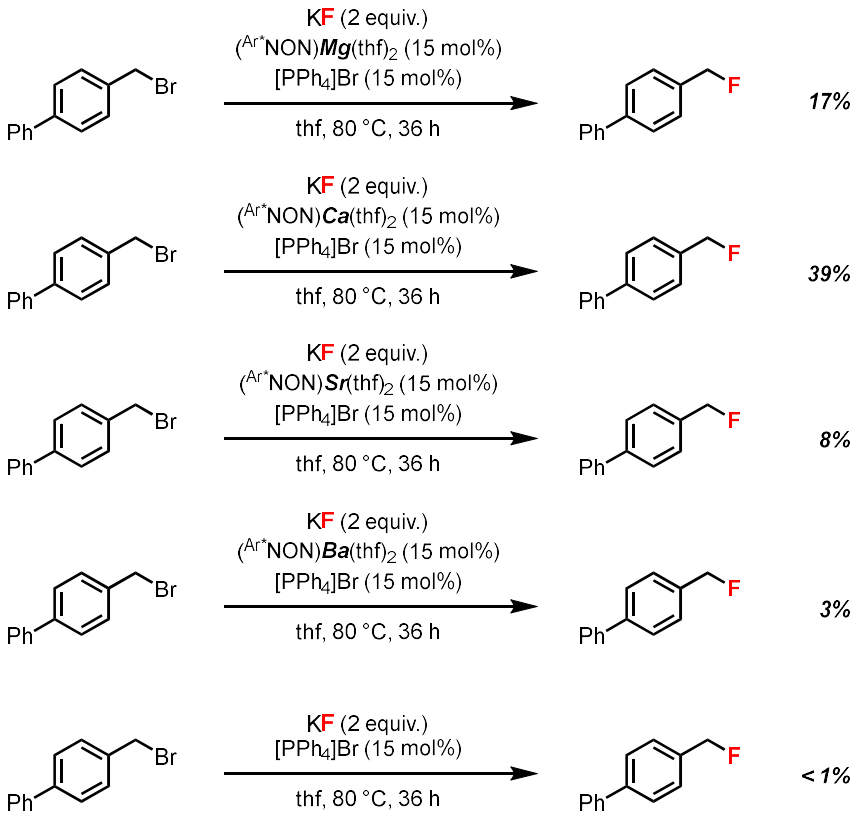


Figure S 20 *Initial scoping on the effect of group two metal on the (^{Ar*}NON)AE(thf)$_2$ catalysed fluorination of alkyl bromides. 4-(bromomethyl)biphenyl was selected as model substrate (1 equiv., 0.02 mmol) and reacted with KF (2 equiv.) in the presence of PPh_4Br (15 mol%) and (^{Ar*}NON)AE(thf) (15 mol%, or for the control: 0 mol%) in thf-d_8 (0.5 mL). All reactions were performed in a J-Young NMR tube at 80 °C. All yields were determined by quantitative ^{19}F NMR spectroscopy with PhF (5 µL) as internal standard. Calcium demonstrated by far the best catalytic performance as compared to other group two metals (or the absence of any (^{Ar*}NON)AE(thf)$_2$) and thus was selected for further studies.*

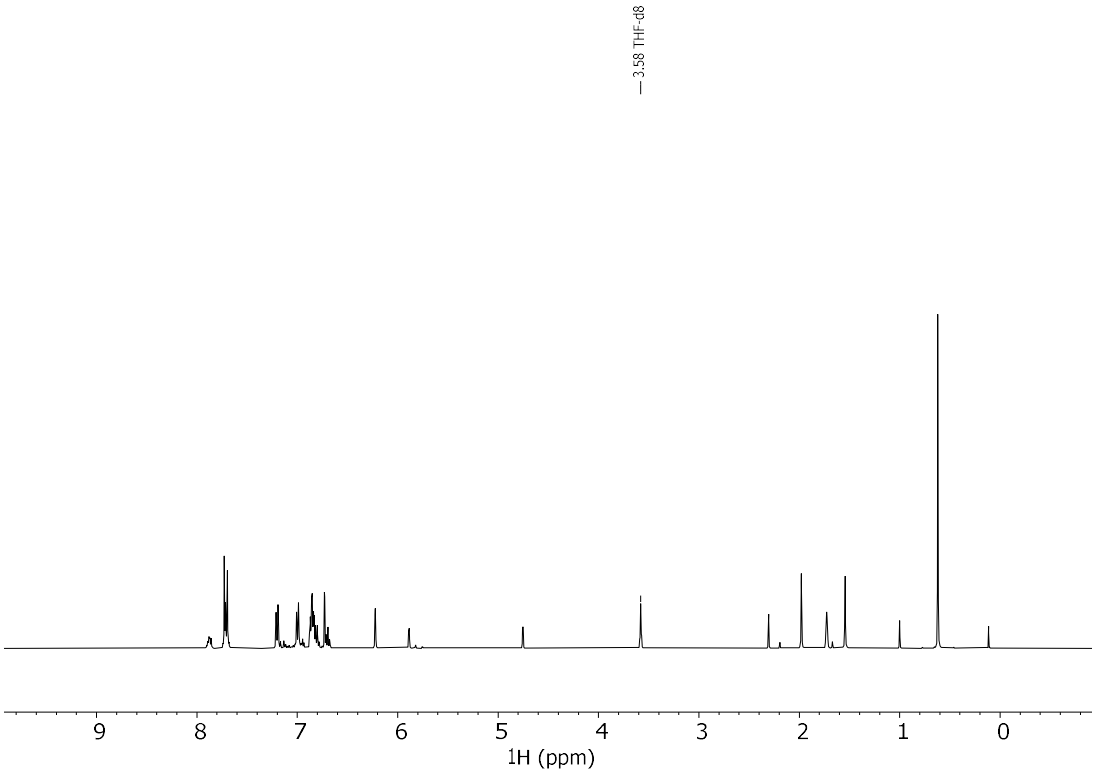


Figure S 21 *^{1}H NMR spectrum of the in-situ formation of **8**-PPh_4 from **1** and $[PPh_4]Br$ in thf-d_8 at RT.*

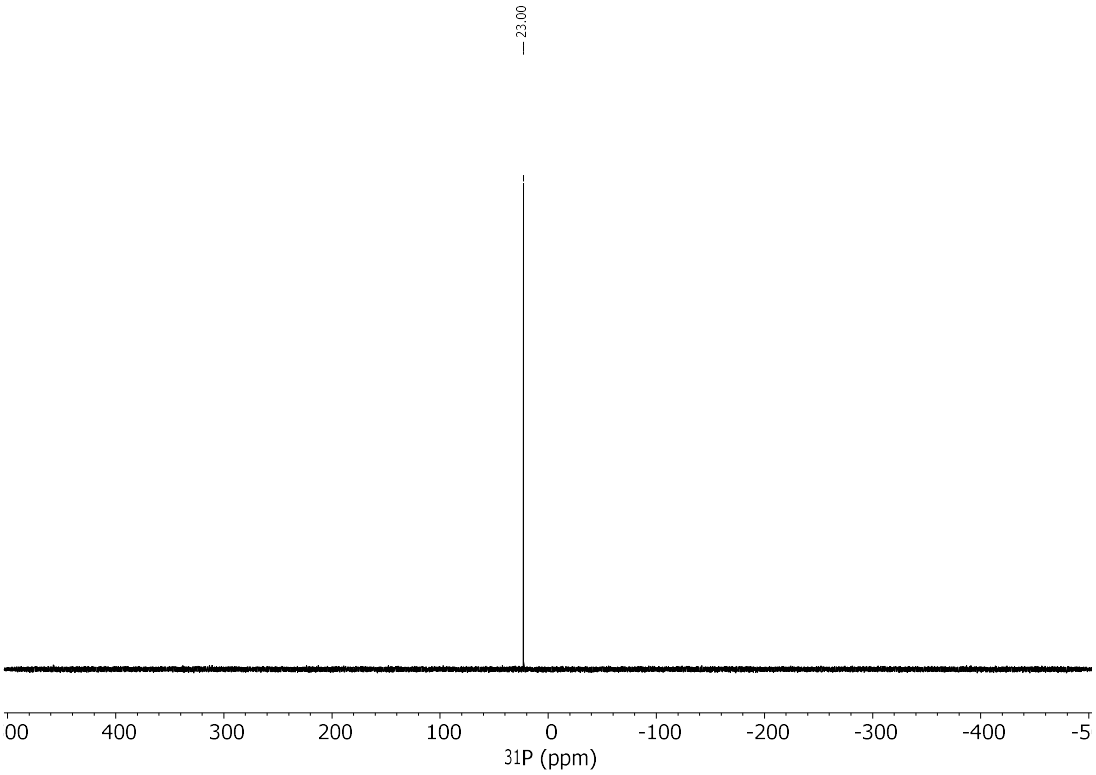


Figure S 22 *^{31}P NMR spectrum of the in-situ formation of **8**-PPh_4 from **1** and $[PPh_4]Br$ in thf-d_8 at RT.*

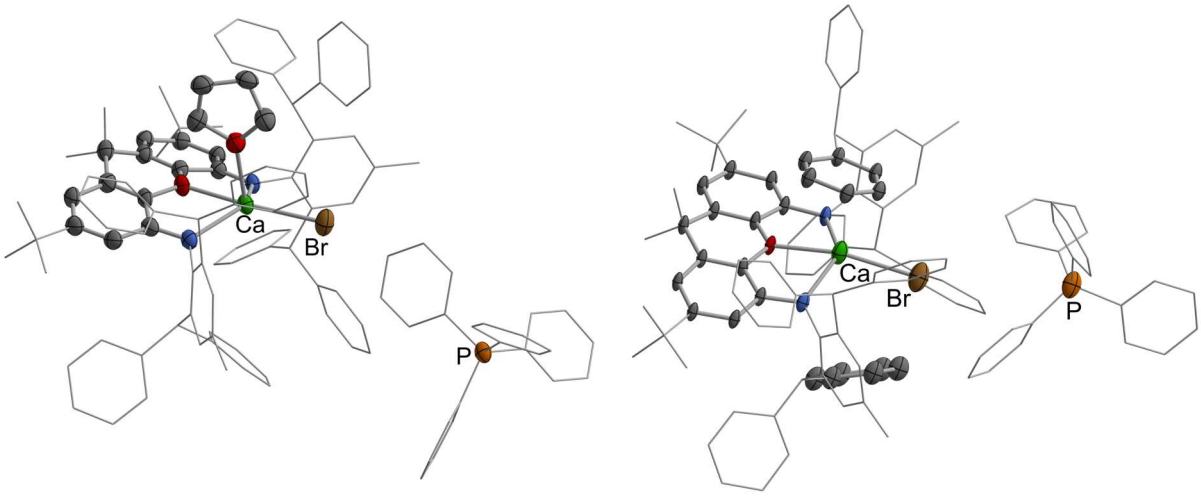


Figure S 23. *Molecular structures of [PPh$_4$][(^{Ar*}NON)CaBr(thf)] (**8**-PPh$_4$-thf, left) and [PPh$_4$][(^{Ar*}NON)CaBr] (**8**-PPh$_4$-□, right) in the solid state both grown from saturated thf/hexane solutions, as determined by X-ray crystallography. Thermal ellipsoids set at the 50% level. Hydrogen atoms, solvate molecules and second disorder components omitted, and selected fragments shown in wireframe format for clarity. The structure of **8**-PPh$_4$-□ is displayed for connectivity purposes only.*

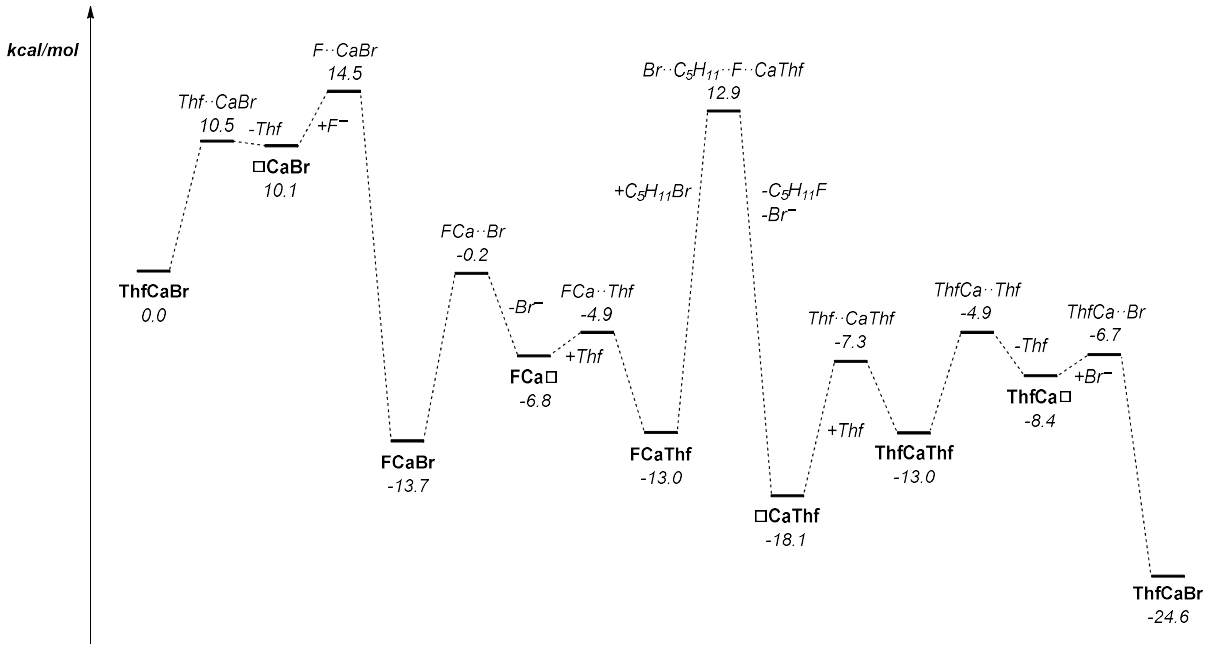


Figure S 24 *Mechanism for the calcium-catalysed conversion of 1-bromopentane ($C_5H_{11}Br$) to 1-fluoropentane ($C_5H_{11}F$) according to quantum-chemical calculations. Complexes are abbreviated as XCaY with X and Y denoting the axial and equatorial position, respectively. Intermediates are bolded and transition states italicized with XCa··Y or X··CaY denoting the group that undergoes leaving/addition. All energies in kcal/mol with respect to ThfCaBr.*

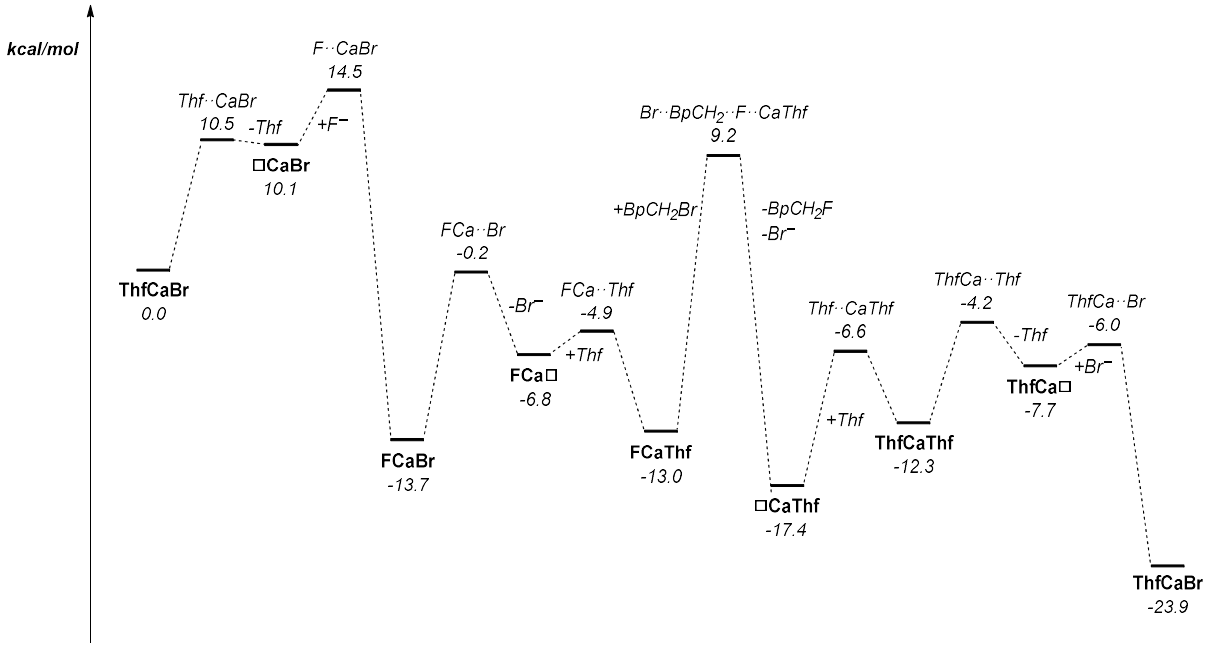
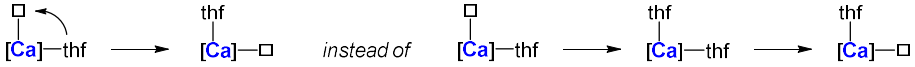


Figure S 25 *Mechanism for the calcium-catalysed conversion of 4-(bromomethyl)biphenyl ($BpCH_2Br$) to 4-(fluoromethyl)biphenyl ($BpCH_2F$) according to quantum-chemical calculations. Complexes are abbreviated as XCaY with X and Y denoting the axial and equatorial position, respectively. Intermediates are bolded and transition states italicized with XCa··Y or X··CaY denoting the group that undergoes leaving/addition. All energies in kcal/mol with respect to ThfCaBr.*

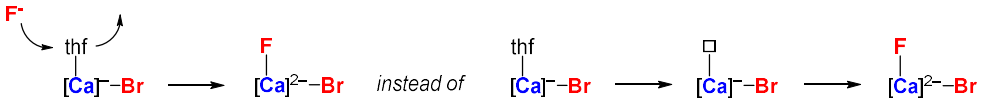
Quantum chemical exploration of alternative mechanisms

Additional quantum chemical analyses were performed to probe alternative mechanisms to those outlined in **Figures S24-25**. Specifically, regarding the possibility for concerted ligand exchange at calcium, key steps in the proposed cycle were re-examined and the respective barriers for processes occurring via concerted processes versus a stepwise dissociative/associative mechanism were compared. In all cases for which transition states could be determined, the energy barrier for the concerted process was found to be higher (the calculated difference for the concerted process as compared to the original mechanism is noted in parentheses):

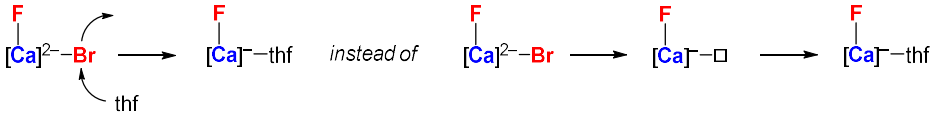
- thf Exchange between axial and equatorial sites (+17.3 kcal mol^{-1})



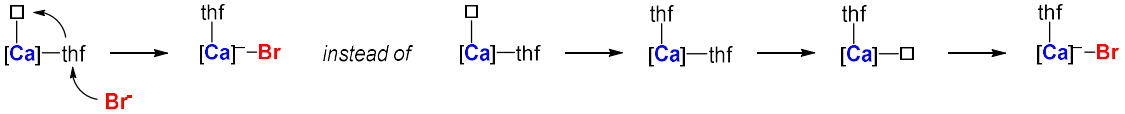
- F-/thf exchange (+8.4 kcal mol^{-1})



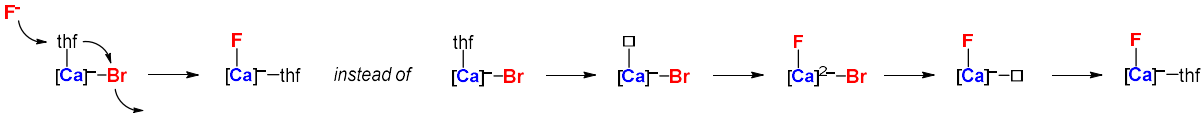
- thf/Br- exchange (+19.0 kcal mol^{-1})



- Br association and thf migration (no transition state found; all attempts resulted in the incoming thf ligand moving away from the coordination sphere instead)



- F-/Br- exchange with thf migration (+7.2 kcal mol^{-1})



General procedure

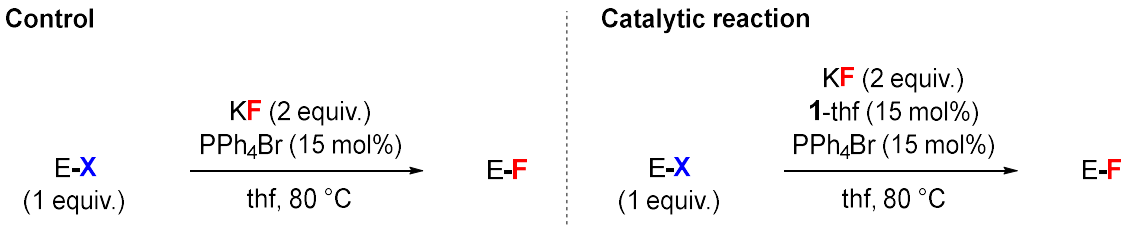


Figure S 26 *Reaction scheme for the calcium-catalysed fluorination of alkyl bromides (1 equiv., 0.02 mmol) by KF (2 equiv.) in the presence of PPh_4Br (15 mol%) and (^{Ar*}NON)Ca(thf) (15 mol%, or for the control: 0 mol%) in thf-d_8 (0.5 mL). All reactions were performed in a J-Young NMR tube at 80 °C. The overall reaction corresponds to KF(s) + E–X → KX(s) + E–X. All products matched characterization reported here or in literature[14,16]. All yields were determined by quantitative ^{19}F NMR spectroscopy with PhF (5 µL) as internal standard. Selected examples are given in* ***Figure S 27****-****Figure S 30****.*

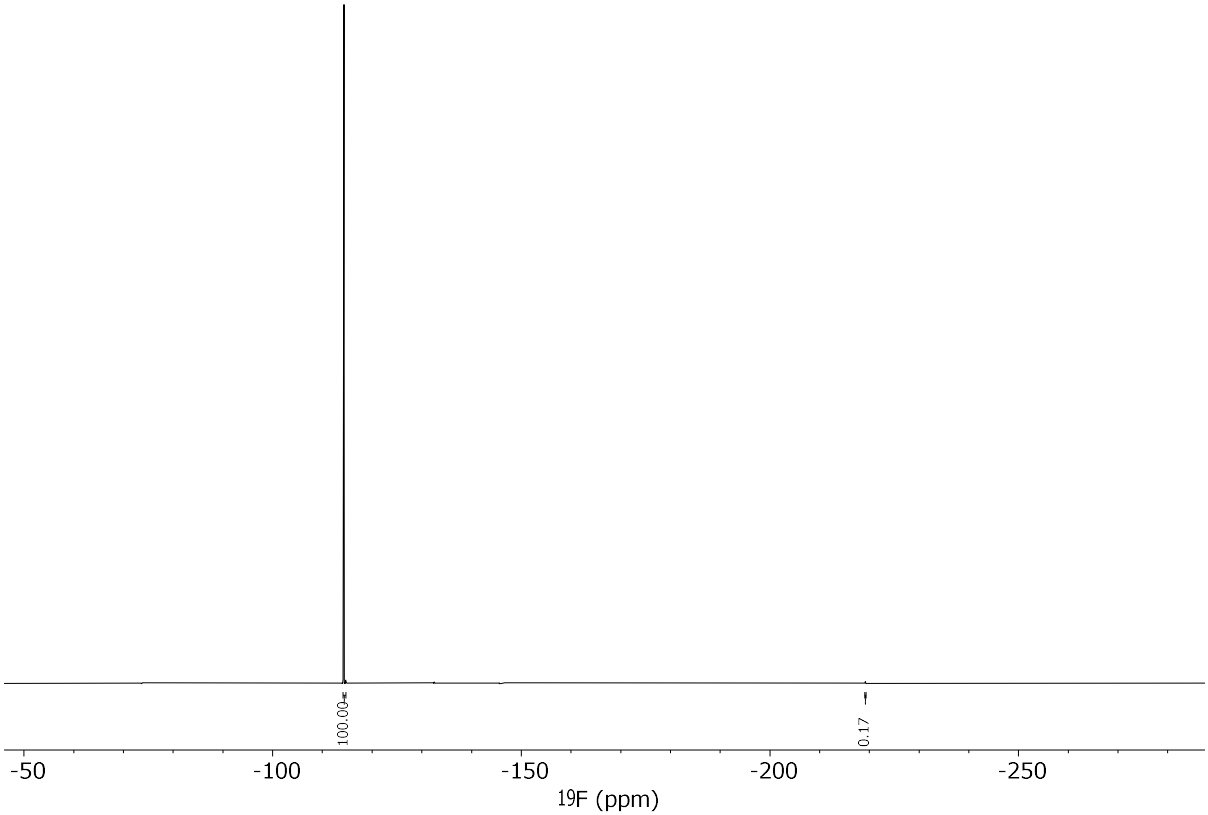


Figure S 27 *Quantitative ^{19}F NMR spectrum for the control reaction of 1-bromopentane with KF in the absence of **1**-thf after 5 days at 80 °C (<0.5% 1-fluoropentane).*

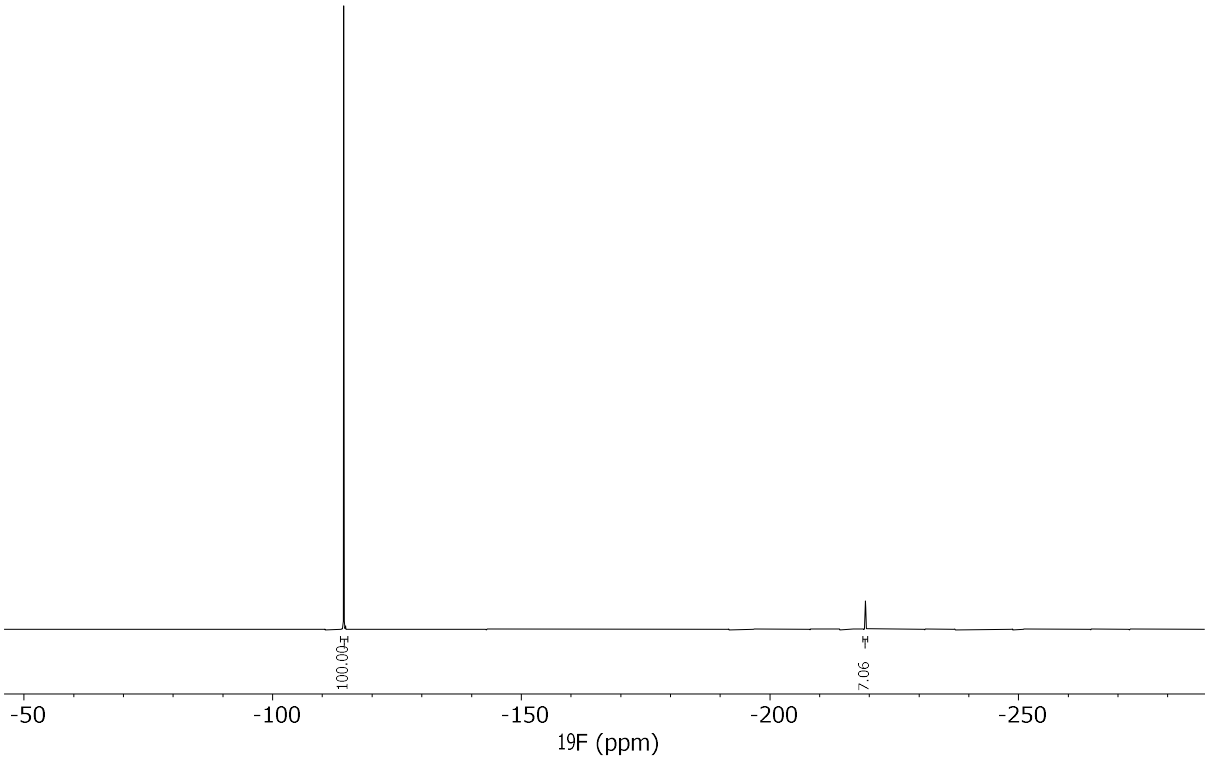


Figure S 28 *Quantitative ^{19}F NMR spectrum for the calcium-catalysed reaction of 1-bromopentane with KF after 25 days at 80 °C (19% 1-fluoropentane).*

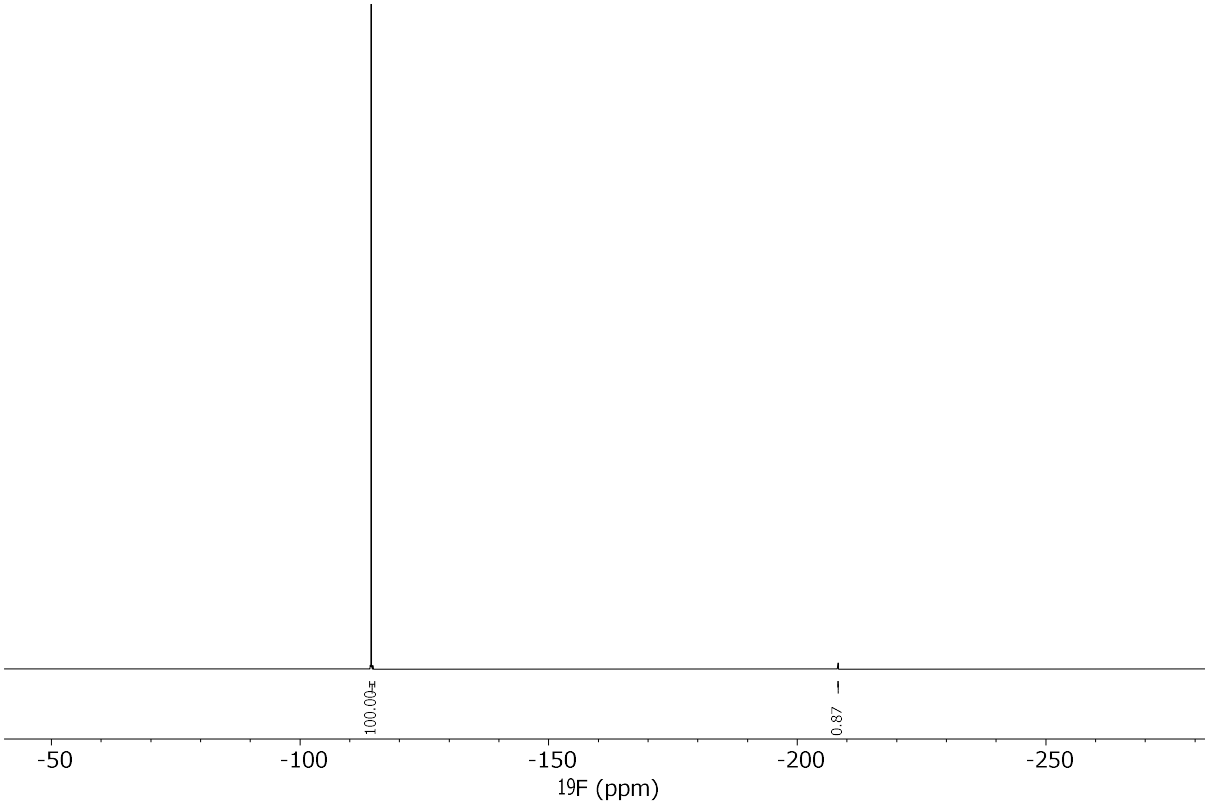


Figure S 29 *Quantitative ^{19}F NMR spectrum for the control reaction of 4-(bromomethyl)biphenyl with KF in the absence of **1**-thf after 5 days at 80 °C (2% 4-(fluoromethyl)biphenyl).*

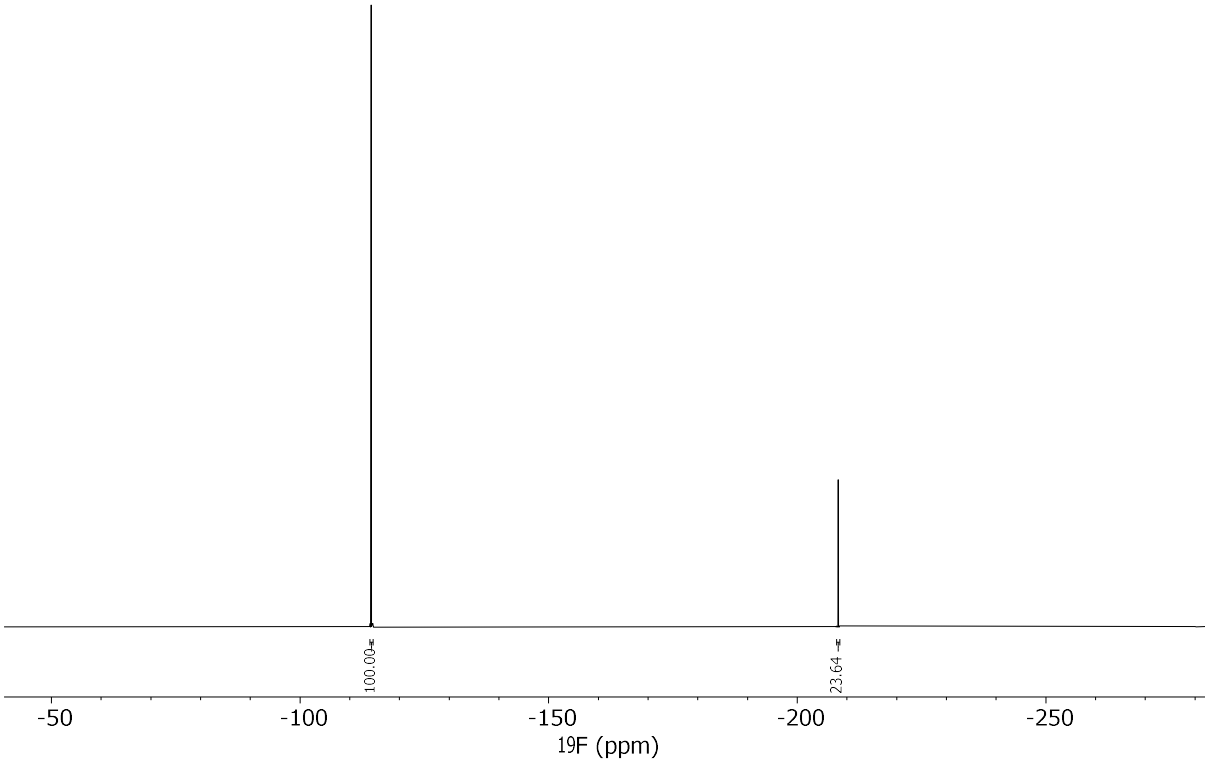


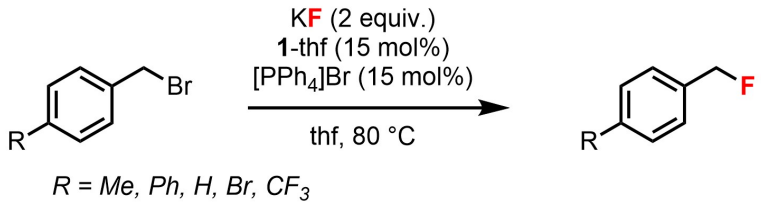
Figure S 30 *Quantitative ^{19}F NMR spectrum for the calcium-catalyzed reaction of 4-(bromomethyl)biphenyl with KF after 5 days at 80 °C (62% 4-(fluoromethyl)biphenyl).*

Hammett analysis and kinetic isotope effect study

To probe the mechanism of the reaction from the perspective of the electrophile (i.e. S_N1-, S_N2-, or metathesis-like pathways), both quantum mechanical calculations and physical organic methods were employed. For the latter, both Hammett analysis and a kinetic isotope effect study were performed as described below. In conclusion, all three methods corroborate a mechanism that from the perspective of 1-bromopentane resembles a classical S_N2 pathway.

Hammett analysis

In addition to the biphenyl model substrate, 4 additional substrates were chosen varying from strongly electron withdrawing to moderately electron donating (due to product instability, strongly electron donating groups as methoxy and dimethylamine groups were omitted)[17] in the form of $-CF_3$ (σ_P = 0.54), -Br (σ_P = 0.23), -H (σ_P = 0.00), -Me (σ_P = -0.17).



Given the heterogeneous nature of the reaction, all substrates were performed in duplicate (**Figure S 31**). The rate constant for each substrate was then determined from the averaged initial rate of each of the two runs (**Figure S 32**) and used to construct the Hammett plot in **Figure S 33**. The rho value that can be determined from the reaction is +0.16 ± 0.16. The small positive value around zero implies that the mechanism is unlikely to be S_N1 type in nature (for which a large negative value would be expected) and is much more in line with a an S_N2 type mechanism with little-to-no charge build up during the transition state in the rate-determining step.

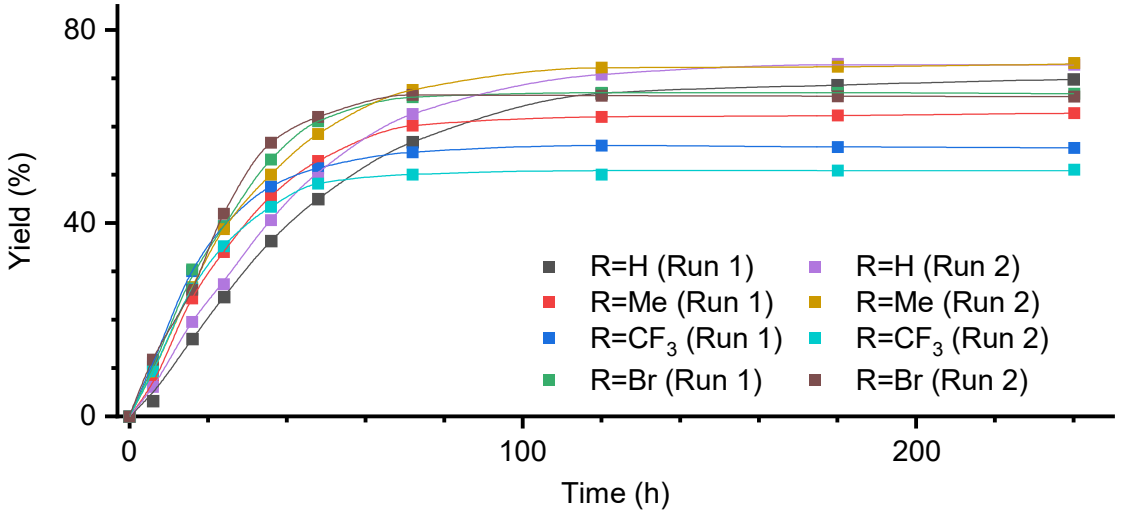


Figure S 31 *Kinetic profiles of the reaction for the catalytic fluorination for 4-R benzyl bromides performed according to the general procedure described in* ***Figure S 26****.*

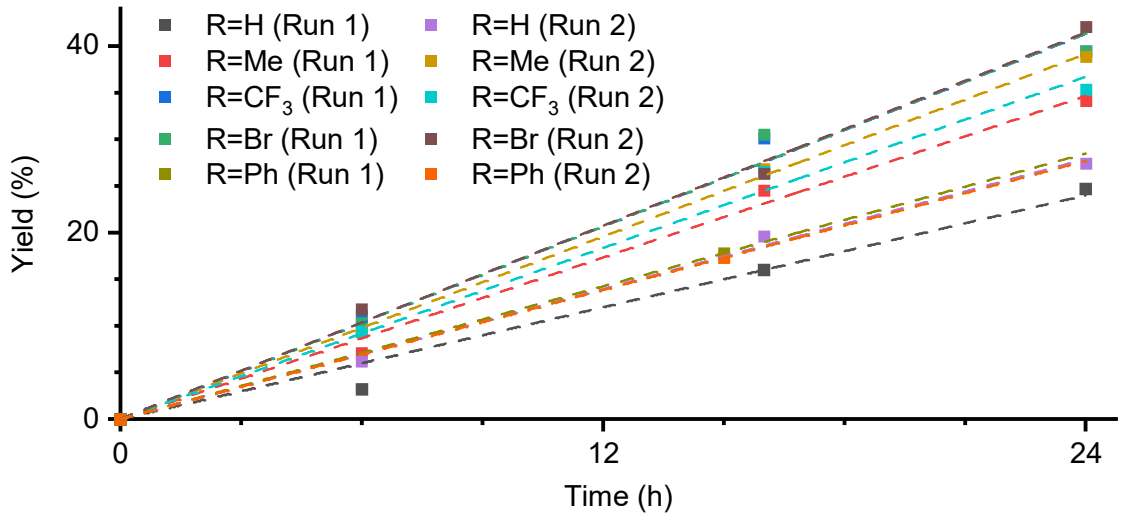


Figure S 32 *Linear fit for the initial rates of the reaction for the kinetic traces in* ***Figure S 31****.*

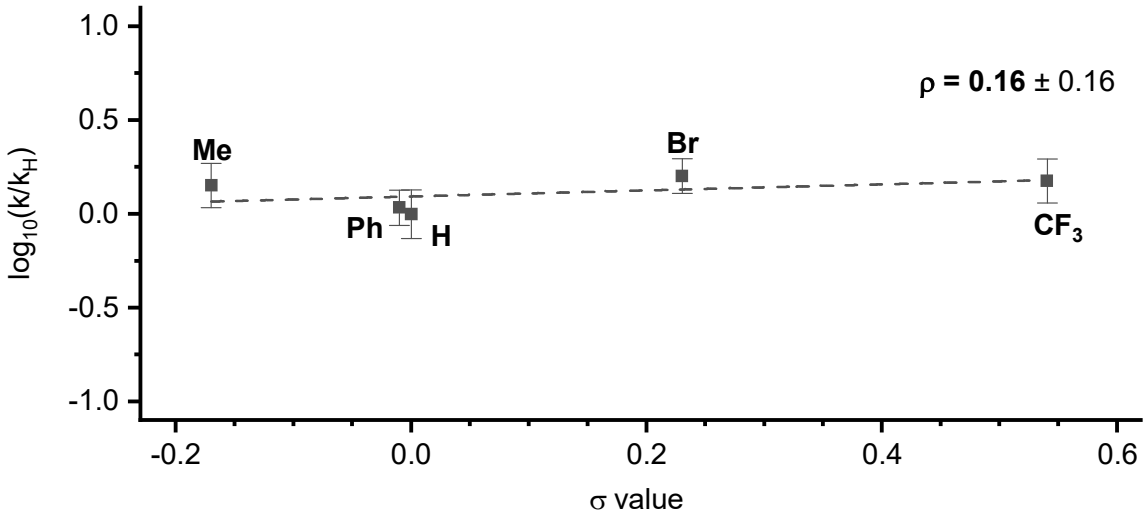
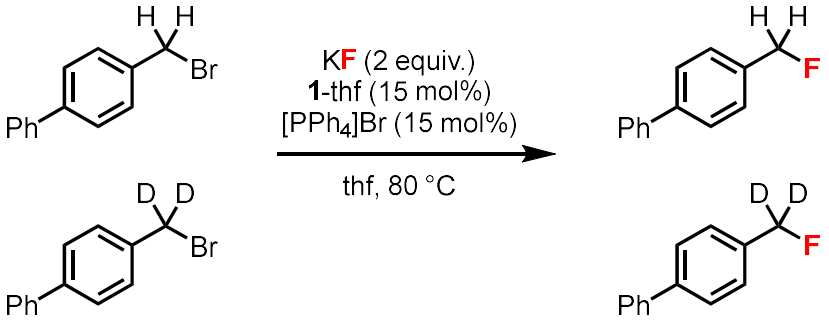


Figure S 33 *Hammett plot for the catalytic fluorination reactions following from* ***Figure S 31*** *and* ***Figure S 32****. For each substrate, the rate constants (k) of the two runs were averaged and subsequently normalized by the averaged rate constant for benzyl bromide (k_H) and plotted as the logarithm versus the respective sigma parameter with error bars representing a 2 sigma deviation, as derived from the two kinetic runs. Linear regression of the line results in a slope (ρ value) of 0.16 with a standard error of 0.16.*

Kinetic isotope effect (KIE) study

To limit experimental error and to assure both the protio- and deuterio-substrate are probed under identical reaction conditions (deemed especially important for this heterogeneous catalytic reaction), an intermolecular *competition* secondary α-KIE experiment (cf. a *parallel* KIE experiment) was performed, following the general procedure described above with 0.01 mmol 4-(bromomethyl)-biphenyl and 0.01 mmol 4-(bromo-d_2-methyl)-biphenyl:[18]



For a first order reaction in A resulting in product P, the following rate equations and mass balance can be set up:

$$\frac{\partial[A(t)]}{\partial t} = -k[A] \qquad \frac{\partial[P(t)]}{\partial t} = +k[A]\,[A(t)] + [P(t)] = [A(0)] + [P(0)]$$

After integration, the following equation can be derived relating $[P(t)]$ to t:

$$\ln\frac{1}{1-X} = kt \qquad \text{with } X = \frac{[P(t)]}{[A(0)]}$$

Letting $[A_H(0)]$ and $[A_D(0)]$ denote the substrate concentrations at $t = 0$, $[P_H(t)]$ and $[P_H(t)]$ the product concentrations at time t, and X_H and X_D the yields at time t of the respective analogues as determined by quantitative ^{1}H and ^{19}F NMR spectroscopy against the fluorobenzene internal standard, these equations can be used to determine k_H and k_D by plotting $ln\frac{1}{1-X}$ versus t for both the protio- and deuterio-analogues, respectively:

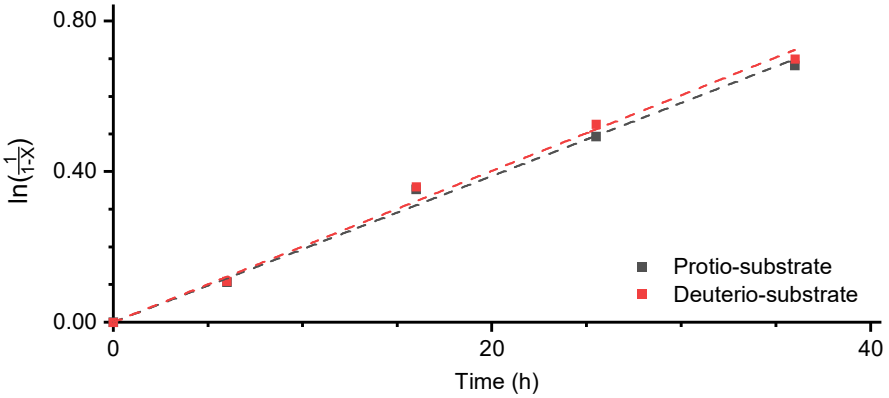


Figure S 34 *Plot of $ln\frac{1}{1-X}$ versus time for the protio- and deuterio-analogue. The slopes of a linear fit with corresponding errors result in $k_H = 1.94(\pm0.05)\cdot10^{-2}$ h^{-1} and $k_D = 2.01(\pm0.05)\cdot10^{-2}$ h^{-1} and thus a KIE of 0.97 ± 0.03. Points after 36 h were omitted due deviation from 1st order behaviour attributed to catalyst deactivation (see **Figure S 35** for a fit based on initial rates without assuming 1st order behaviour).*

From the values of k_H = 1.94(±0.05)·10^{-2} h^{-1} and k_D = 2.01(±0.05)·10^{-2} h^{-1}, then the KIE can be determined as:

$$KIE = \frac{k_H}{k_D} = 0.97 \pm 0.03$$

A secondary α-KIE around 1.0 is not consistent with an S_N1 type mechanism (for which a higher KIE of ~1.1-1.3 would be expected); the turnover-limiting step is more in line with an S_N2 type mechanism.

It should be noted that the analysis above assumes the reaction to be first order in alkyl bromide. However, a similar KIE of 0.98 ± 0.03 was obtained using the method of initial rates, for which this assumption is not required:

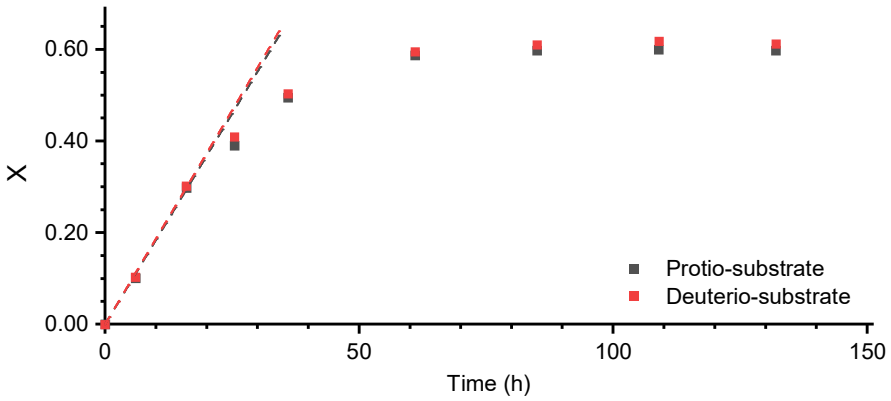
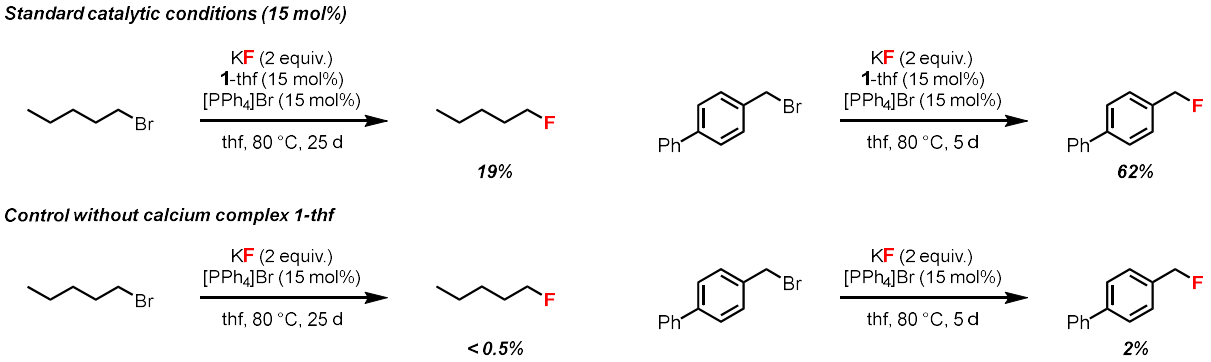


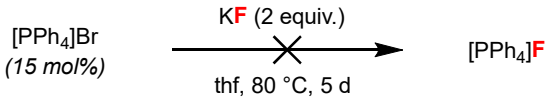
Figure S 35 *Plot of X (i.e. product yield) versus time for the protio- and deuterio-analogue. The initial rates result in a KIE of 1.84(±0.04)·10^{-2} h^{-1} / 1.87(±0.04)·10^{-2} h^{-1} = 0.98 ± 0.03 as determined from the slopes of the linear fits with corresponding errors. Points after 16 h were omitted from the fit due deviation from linear behaviour.*

Investigations into [PPh$_4$]F as (in-situ generated) fluoride source

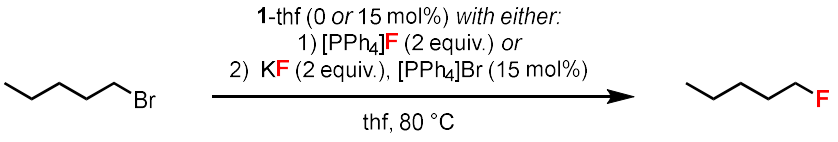
To investigate the possibility of [PPh$_4$]F acting as the main (in-situ generated) fluoride source, a variety of control reactions were performed. First of all, identical reactions in the presence and absence of calcium complex **1**-thf demonstrates that [PPh$_4$]Br by itself does not act as a competent phase transfer agent in the fluorination of alkyl bromides and thus signifies the importance of the calcium complex in the fluorination (see also **Fig. 3** and **Figure S 26**; note that [PPh$_4$]Br is included in both reactions):



Noteworthy, the absence of any [PPh$_4$]F in the control reactions (as judged by the absence of (doublet) signals in ^{19}F and ^{31}P NMR spectroscopy as would be expected for the thf-soluble [PPh$_4$]F) demonstrates that its formation from KF and [PPh$_4$]Br is unfavorable under the reaction conditions applied. Also in the absence of alkyl bromides, no [PPh$_4$]F was detected by the reaction of KF with [PPh$_4$]Br, further disproving [PPh$_4$]F acting as the (main) fluoride source:



Lastly, a significant acceleration is observed in the presence of calcium complex **1**-thf (cf. the identical reaction without **1**-thf) when replacing KF with [PPh$_4$]F as the fluoride source (**Figure S 36**). It can thus be concluded that even if [PPh$_4$]F would be formed in the catalytic reaction with KF, the reaction rate of [PPh$_4$][(^{Ar*}NON)CaF(thf)] (**2**-PPh$_4$) is significantly higher than for [PPh$_4$]F itself. Moreover, the use of [PPh$_4$]F in these reactions led to a loss of selectivity towards the fluorinated product (versus elimination) both in the presence and absence of **1**-thf (although the incorporation of **1**-thf did lead to a significant improvement in selectivity).



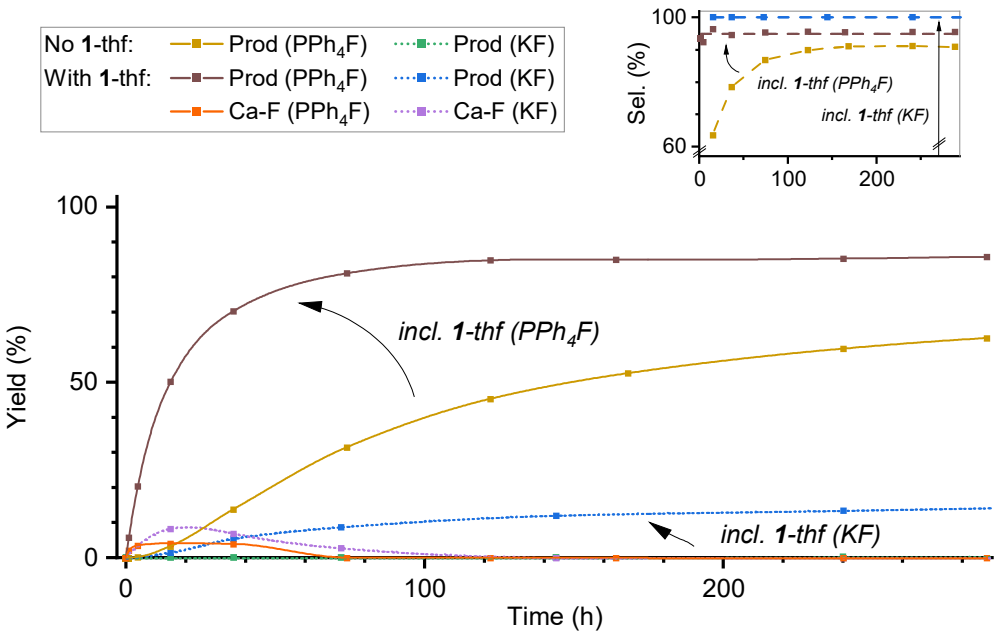


Figure S 36 *Temporal plot for the catalytic fluorination of 1-bromopentane and the corresponding control without* ***1****-thf for either KF (2 equiv.) with [PPh₄]Br (15 mol%) or [PPh₄]F (2 equiv.) as fluoride source (dotted and full lines, respectively) in thf-d₈ (0.5 mL). For both fluoride sources, a significant rate acceleration is observed upon the inclusion of* ***1****-thf. Insert (top right): temporal plot of the selectivity of the reactions towards fluorination (versus elimination), demonstrating that the utilization of [PPh₄]F instead of KF leads to a lower selectivity. Crucially, here the inclusion of* ***1****-thf also does lead to an improvement in selectivity as a result of the higher relative rate of fluorination as compared to the background elimination reaction caused by [PPh₄]F itself. All yields were determined by quantitative ^{1}H and ^{19}F NMR spectroscopy with PhF as internal standard.*

Catalyst decomposition studies

During all catalytic fluorination reactions, quantitative ^{1}H and ^{19}F NMR spectroscopy revealed a gradual decrease in the combined concentration of the two catalytically relevant resting states, [PPh_4][(^{Ar*}NON)CaF(thf)] and [PPh_4][(^{Ar*}NON)CaBr(thf)]. The relative distribution of these species depends on reaction conditions (vide supra), yet their total concentration consistently diminished over time. For instance, catalytic fluorination with a high catalyst loading of 15 mol% and a low initial substrate concentration of 0.04M tips the balance to [PPh_4][(^{Ar*}NON)CaF(thf)] as the predominant resting state with the concentration of this key intermediate decreasing over time as displayed in its kinetic profile (Fig 3E). This depletion correlates with a reduced rate of product formation and ultimately limits overall reaction progress and catalyst turnover number (TON). Upon completion and quenching of the catalytic reaction (e.g. by the addition of a small quantity of water), the ligand framework is observed solely as the protio-ligand $^{Ar*}NONH_2$, indicating that ligand itself stays intact even upon catalyst decomposition.

The stoichiometric reaction of the isolated fluorinating species ([PPh_4][(^{Ar*}NON)CaF(thf)], **2**-PPh_4) with challenging substrates such as 1-bromopentane further corroborates long-term catalyst instability at elevated temperatures in thf. The reaction of **2**-PPh_4 with 1-bromopentane at 80 °C results exclusively in the formation of 1-fluoropentane (60% yield) from the perspective of the electrophile, with the rest of the 1-bromopentane remaining untouched (*vide supra*). From the perspective of the calcium complex, no residual Ca–F species are detected at the end of the reaction and even though the formation 1-fluoropentane from of **2**-PPh_4 is accompanied by an equivalent amount of [PPh_4][(^{Ar*}NON)CaBr(thf)] (matching independently prepared **8**-PPh_4), a significant fraction is converted to $^{Ar*}NONH_2$ (ca. 21%). No other ^{Ar*}NON species were detected by NMR, instead small amounts of insoluble solid were observed which would be consistent with decomposition of **2**-PPh_4 into poorly soluble decomposition products.

The solid decomposition products are believed to be related to the decomposition to the strong thermodynamic sink CaF_2. A key intermediate towards the formation of CaF_2 would be the calcium difluoride complex [PPh_4]$_2$[(^{Ar*}NON)CaF_2] (**3**-(PPh_4)$_2$). The monofluoride complex **2**-PPh_4 immediately reacts with an additional equivalent of PPh_4F in thf to result in the formation of a solid precipitate with ^{1}H and ^{19}F NMR spectroscopy demonstrating the presence of remaining PPh_4F, small amounts of **2**-PPh_4, trace amounts of the targeted difluoride (δ_F = -74.9 ppm), and the formation of $^{Ar*}NONH_2$. The formed solid can be redissolved and characterized in MeCN, where its spectroscopic features match those obtained via independent synthesis in this solvent (*vide supra*). However, also in MeCN, the difluoride exhibits limited solubility and decomposes over time yielding $^{Ar*}NONH_2$, as confirmed by NMR spectroscopy and single-crystal X-ray diffraction of crystals grown from these samples. Consistent with these findings, NMR analysis of catalytic mixtures over time demonstrates the formation of $^{Ar*}NONH_2$. Taken together, these results would support a decomposition pathway in which the formation of the difluoride species, followed by precipitation and/or subsequent degradation, leads to irreversible catalyst deactivation and thus halting catalysis.

Lastly, a decomposition study was conducted under conditions identical to the catalytic reaction but in the absence of any alkyl bromide substrate (**Figure S 37**). Under these conditions, conversion of the bromide complex (formed in-situ from **1**-thf and $[PPh_4]Br$) to the calcium-fluoride analogue **2**-PPh_4 was observed initially, accompanied by the formation of $^{Ar*}NONH_2$ and a decrease in overall mass balance. The formed **2**-PPh_4 slowly decomposes over time, further leading to the formation of $^{Ar*}NONH_2$ and a decrease in overall mass balance accompanied by solid formation, in line with the observations under catalytic conditions. The decomposition is again believed to originate from the formation of insoluble materials and/or decomposition to CaF_2 and secondary species such as $[PPh_4]_2[^{Ar*}NON]$ which then could undergo further decomposition towards $^{Ar*}NONH_2$.

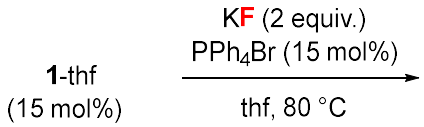


Figure S 37 *Reaction scheme for the catalyst decomposition study under standard catalytic conditions in the absence of alkyl bromide substrate. The reaction was performed using KF (2 equiv.), PPh_4Br (15 mol%), and ($^{Ar*}NON$)Ca(thf) (15 mol%) in thf-d_8 (0.5 mL) in a J-Young NMR tube at 80 °C. Reaction progress and species distribution were monitored by quantitative ^1H and ^{19}F NMR spectroscopy using PhF (5 µL) as an internal standard. The resulting kinetic profile is displayed in* ***Figure S 38****.*

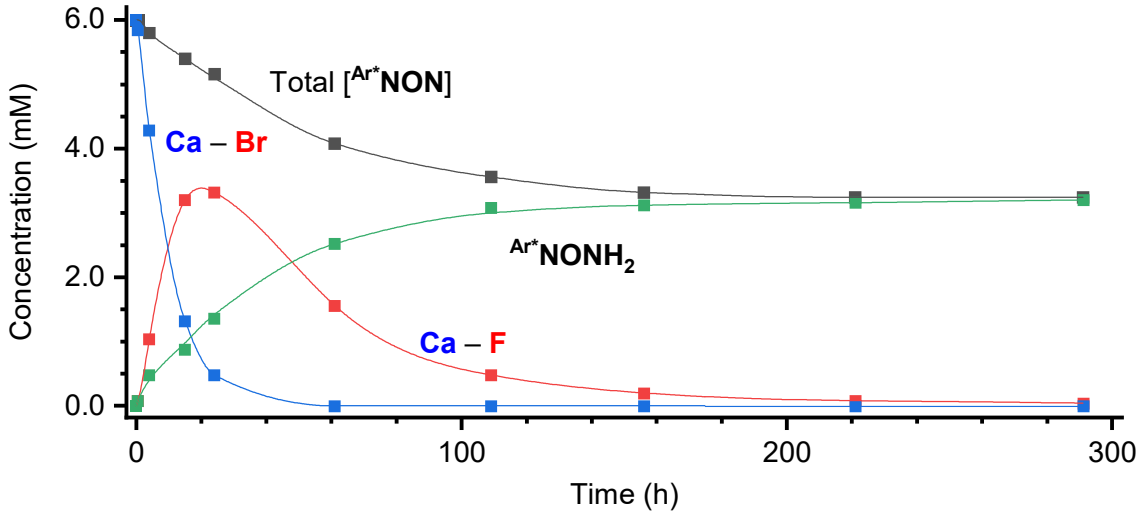


Figure S 38 *Kinetic profiles obtained from the catalyst decomposition study described in* ***Figure S 37****, showing the time-dependent consumption of [$^{Ar*}NONCaBr(thf)$] and, after its formation, [PPh_4][$^{Ar*}NONCaF(thf)$] with the concurrent formation of decomposition products including $^{Ar*}NONH_2$ detected by ^1H NMR.*

Analysis of the divergent reactivity for terminal calcium-fluoride complexes

(See next page)

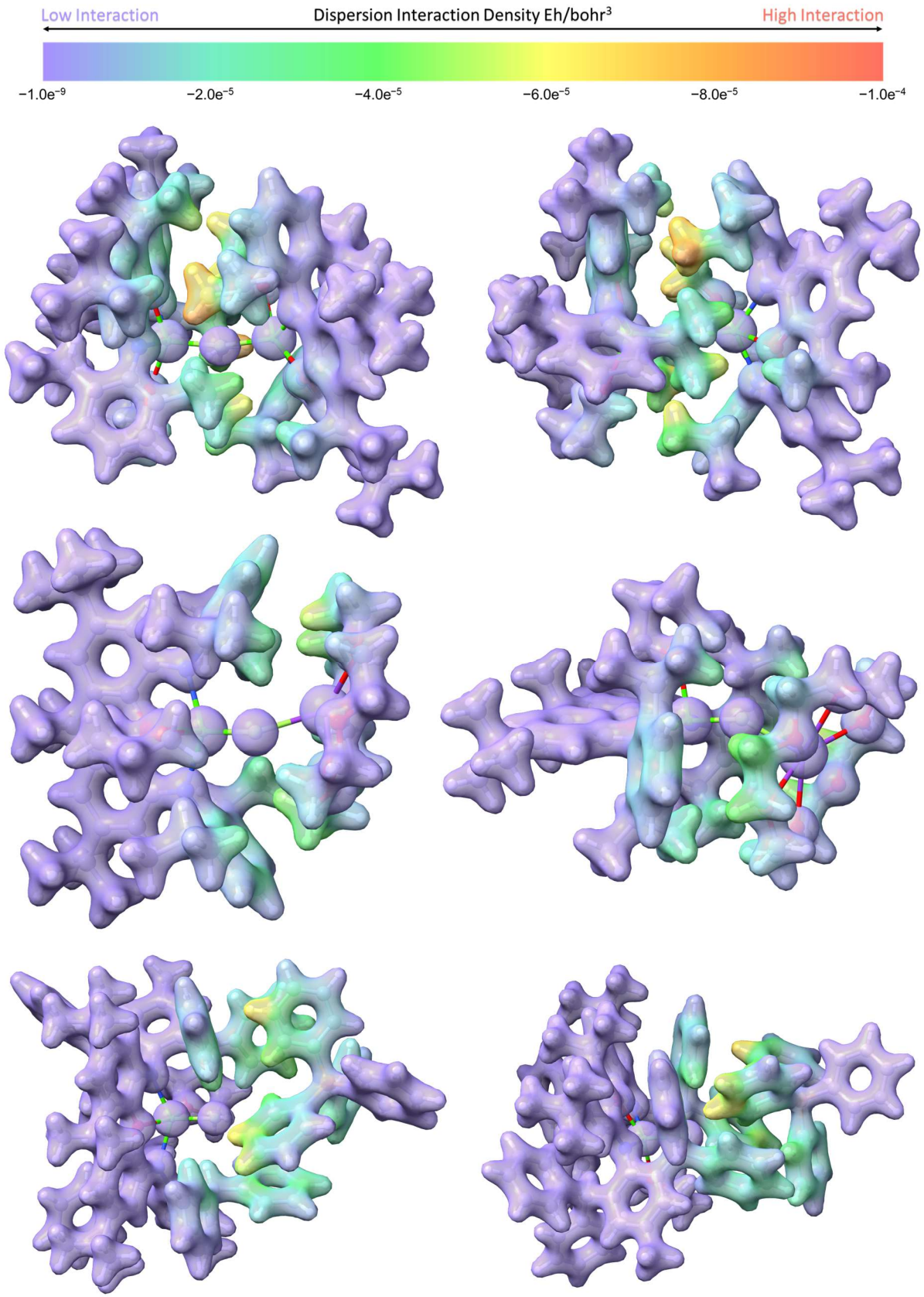


***Figure S 39**. Linear Dispersion Interaction Density (DID) plot showing the strength and location of weak secondary interactions (dispersion forces) as derived from Local Energy Decomposition (LED) analysis. From top to bottom (both left and right): [TMA]$_2$[{(^{Dipp}NON)Ca(μ_2-F)}$_2$], [K(18-crown-6)FCa(thf)(^{Dipp}NON)], and **2**-PPh$_4$. Within **2**-PPh$_4$, strongest interactions are observed between the phenyl rings of [PPh$_4$]$^+$ and [(^{Ar*}NON)]$^{2-}$, respectively.*

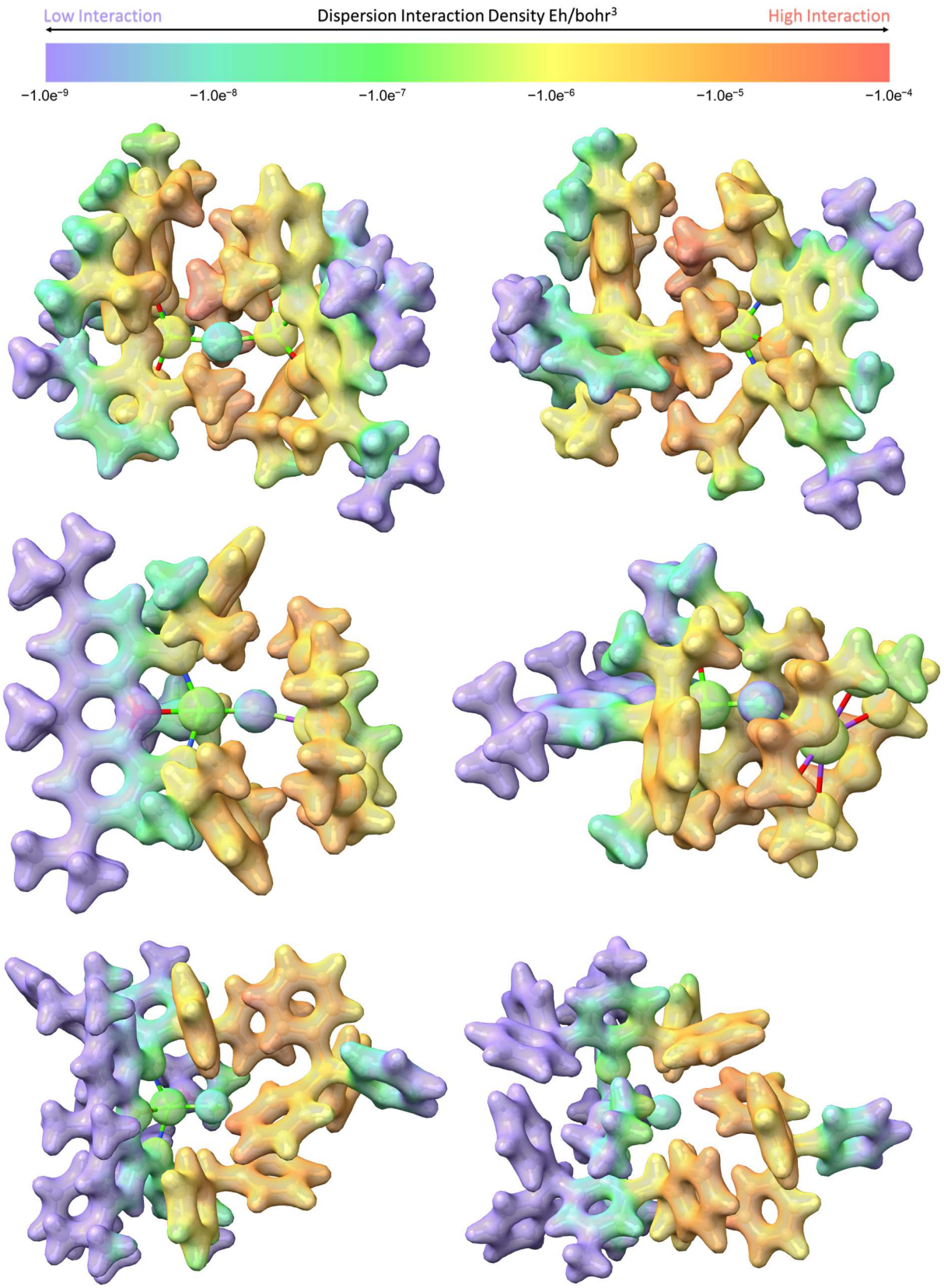


***Figure S 40**. Logarithmic Dispersion Interaction Density (DID) plot showing the strength and location of weak secondary interactions (dispersion forces) as derived from Local Energy Decomposition (LED) analysis. From top to bottom (both left and right): [TMA]$_2$[{(^{Dipp}NON)Ca(μ_2-F)}$_2$], [K(18-crown-6)FCa(thf)(^{Dipp}NON)], and **2**-PPh$_4$. Within **2**-PPh$_4$, strongest interactions are observed between the phenyl rings of [PPh$_4$]$^+$ and [(^{Ar*}NON)]$^{2-}$, respectively.*

3. NMR spectra of synthesized compounds

^{Ar*}NONH$_2$

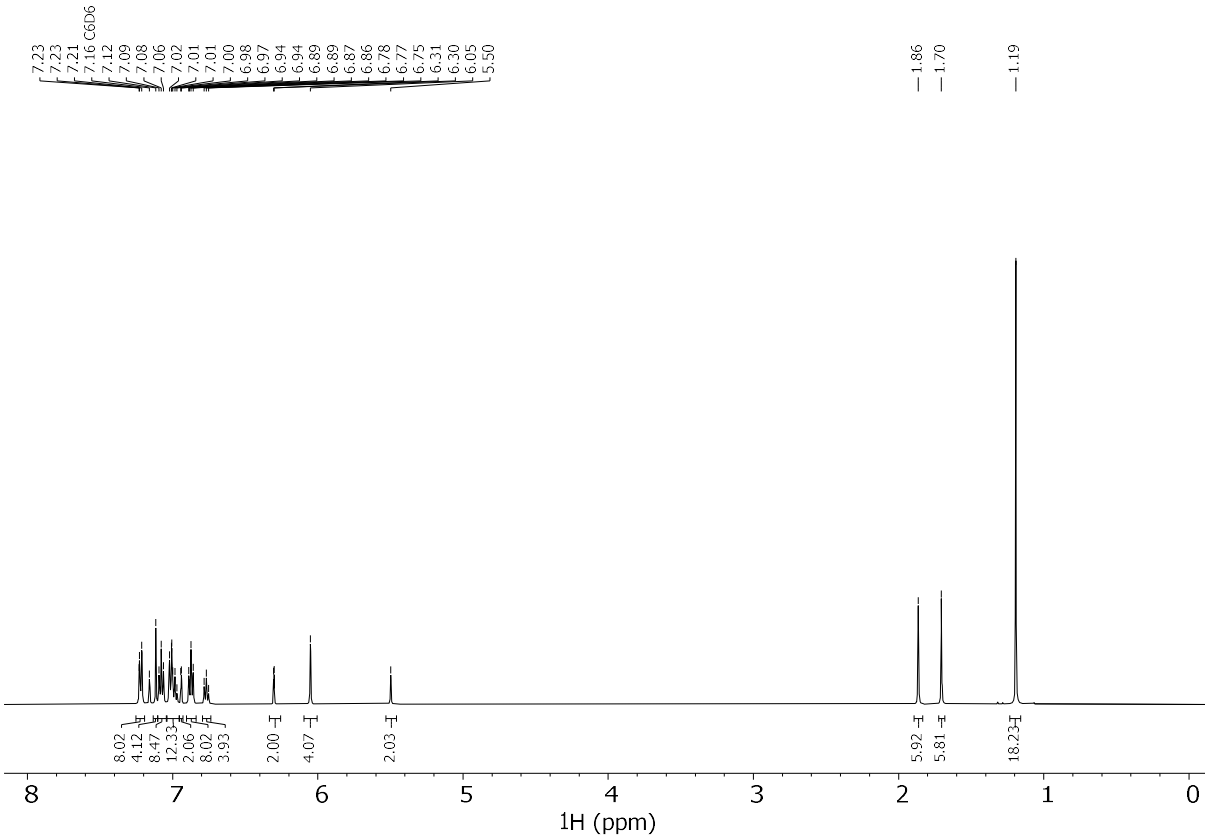


Figure S 41 *^{1}H NMR spectrum of ^{Ar*}NONH$_2$ in C_6D_6 at 298 K.*

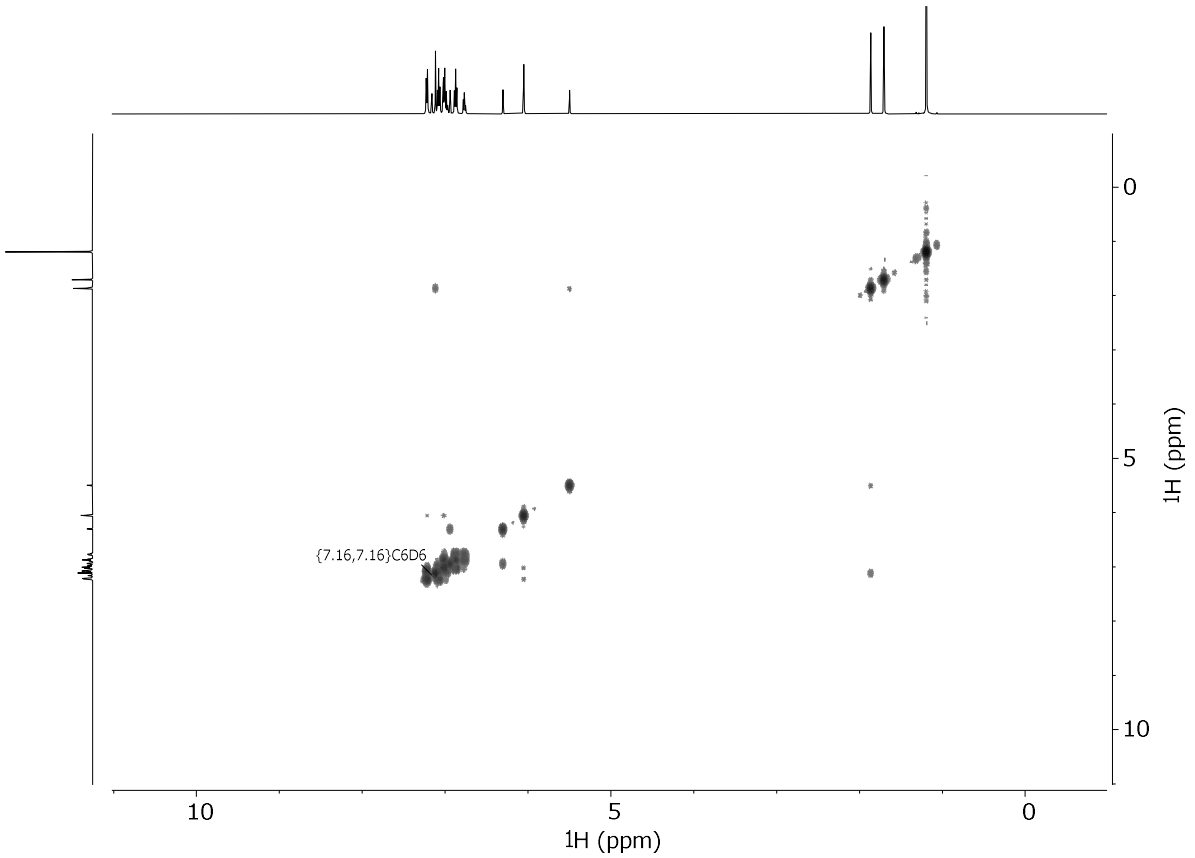


Figure S 42 *^{1}H-^{1}H COSY NMR spectrum of $^{Ar*}NONH_2$ in C_6D_6 at 298 K.*

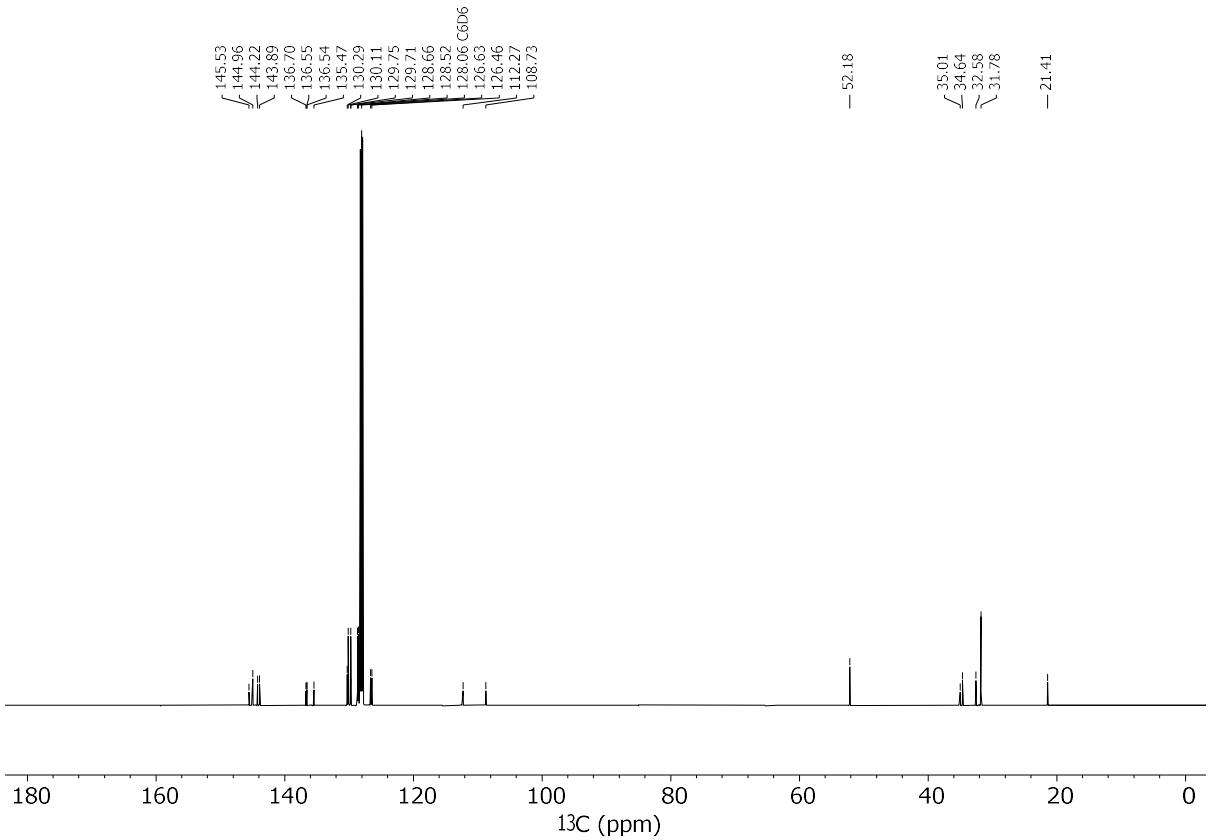


Figure S 43 *$^{13}C\{^1H\}$ NMR spectrum of $^{Ar*}NONH_2$ in C_6D_6 at 298 K.*

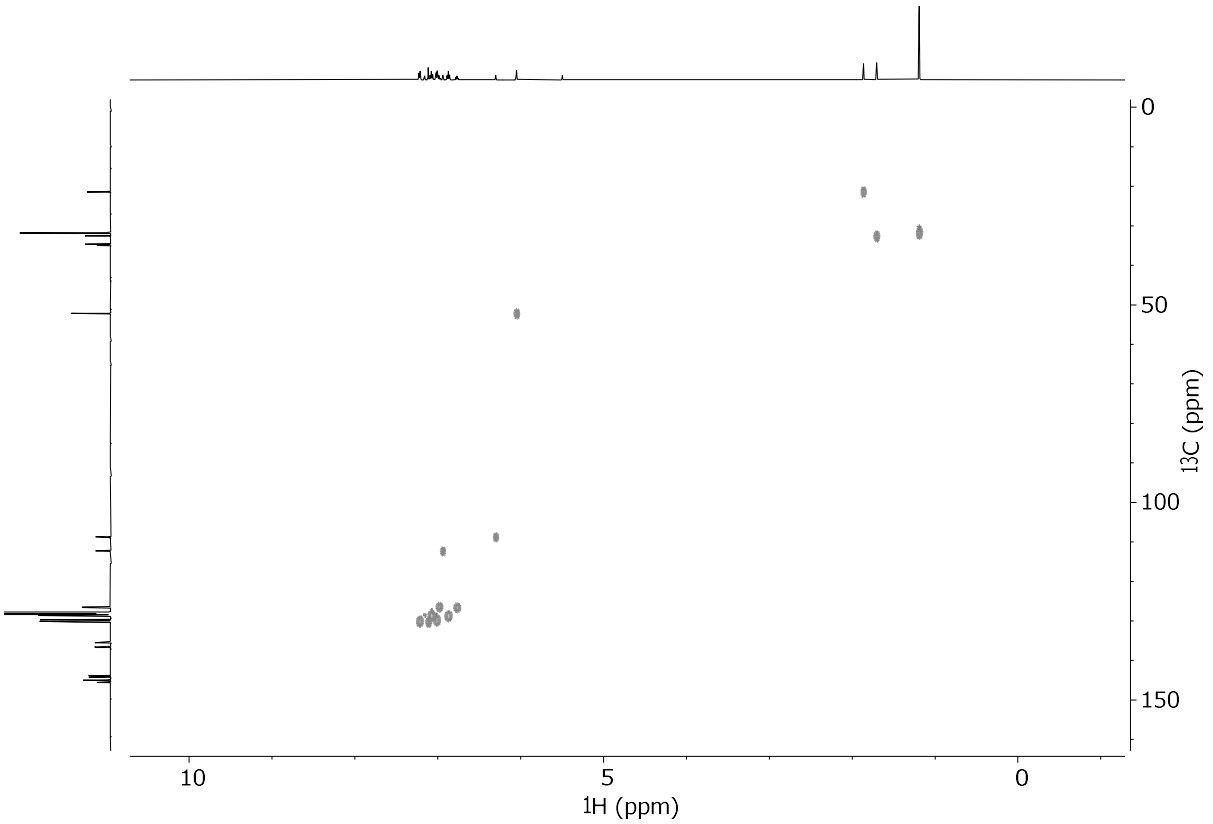


Figure S 44 *^{13}C-^{1}H HSQC NMR spectrum of $^{Ar*}NONH_2$ in C_6D_6 at 298 K.*

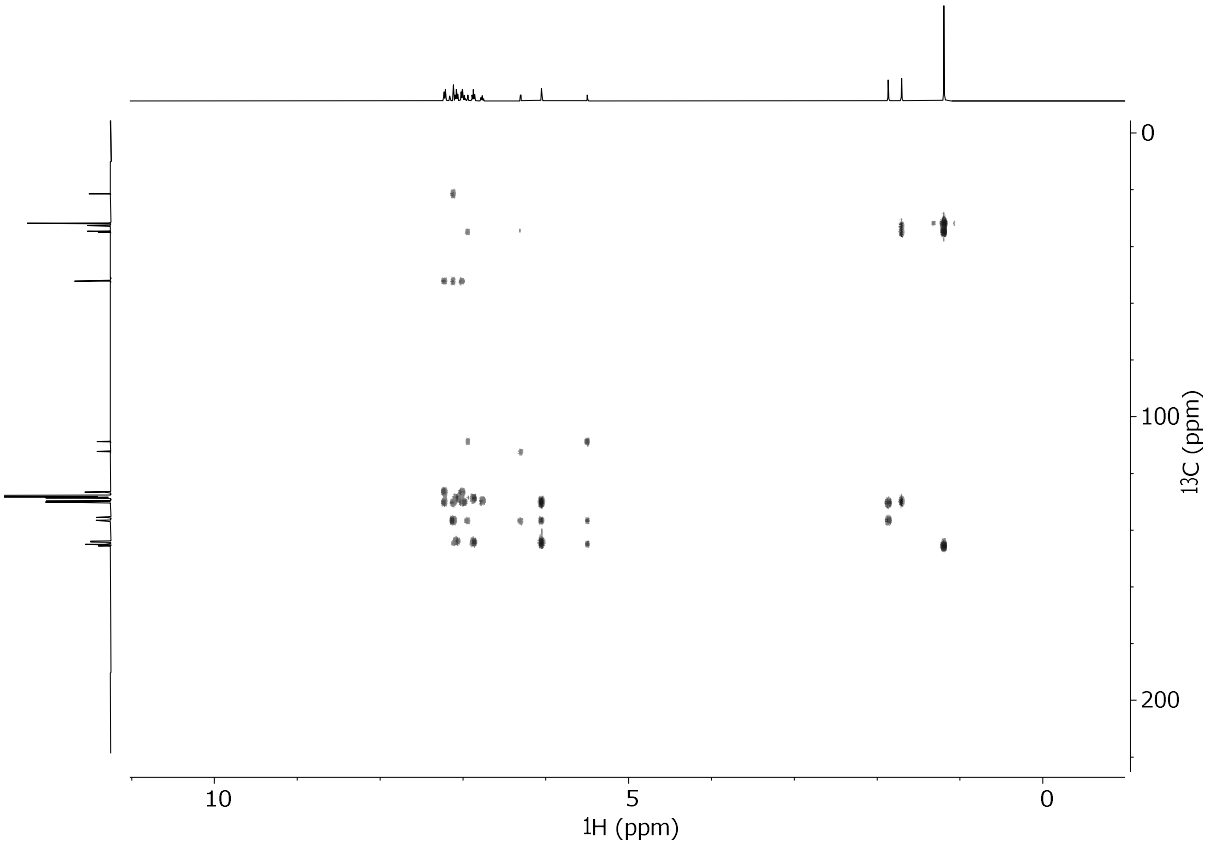


Figure S 45 *^{13}C-^{1}H HMBC NMR spectrum of $^{Ar*}NONH_2$ in C_6D_6 at 298 K.*

^{Ar*}NONK$_2$

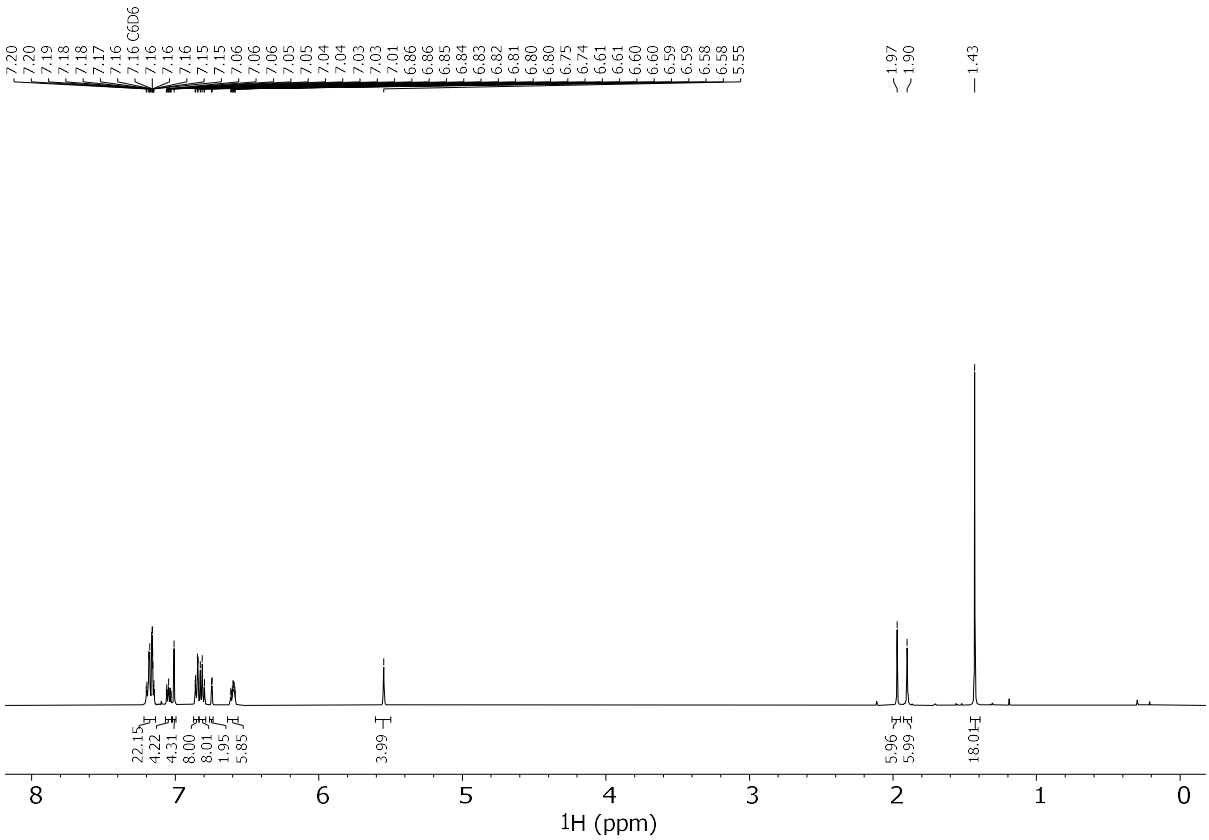


***Figure S 46** ^{1}H NMR spectrum of ^{Ar*}NONK$_2$ in C_6D_6 at 298 K.*

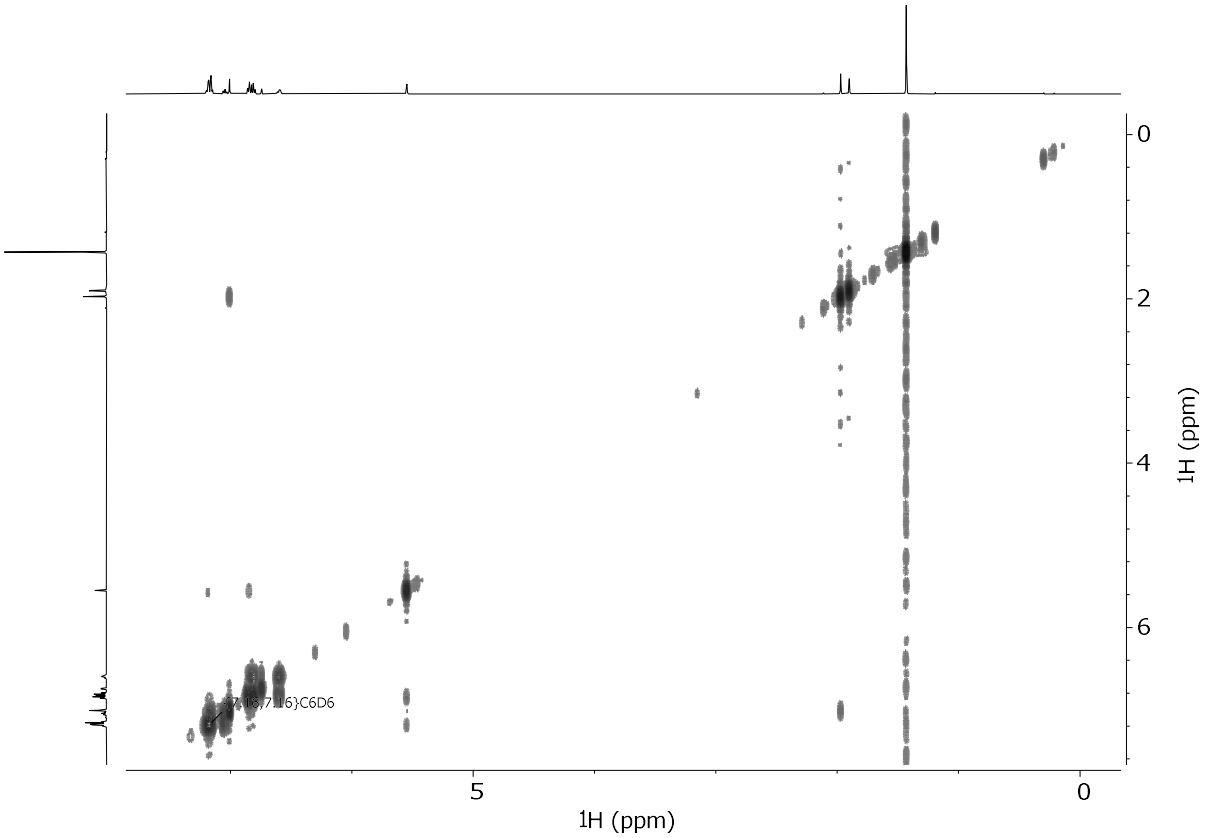


Figure S 47 *^{1}H-^{1}H COSY NMR spectrum of ^{Ar*}NONK$_2$ in C_6D_6 at 298 K.*

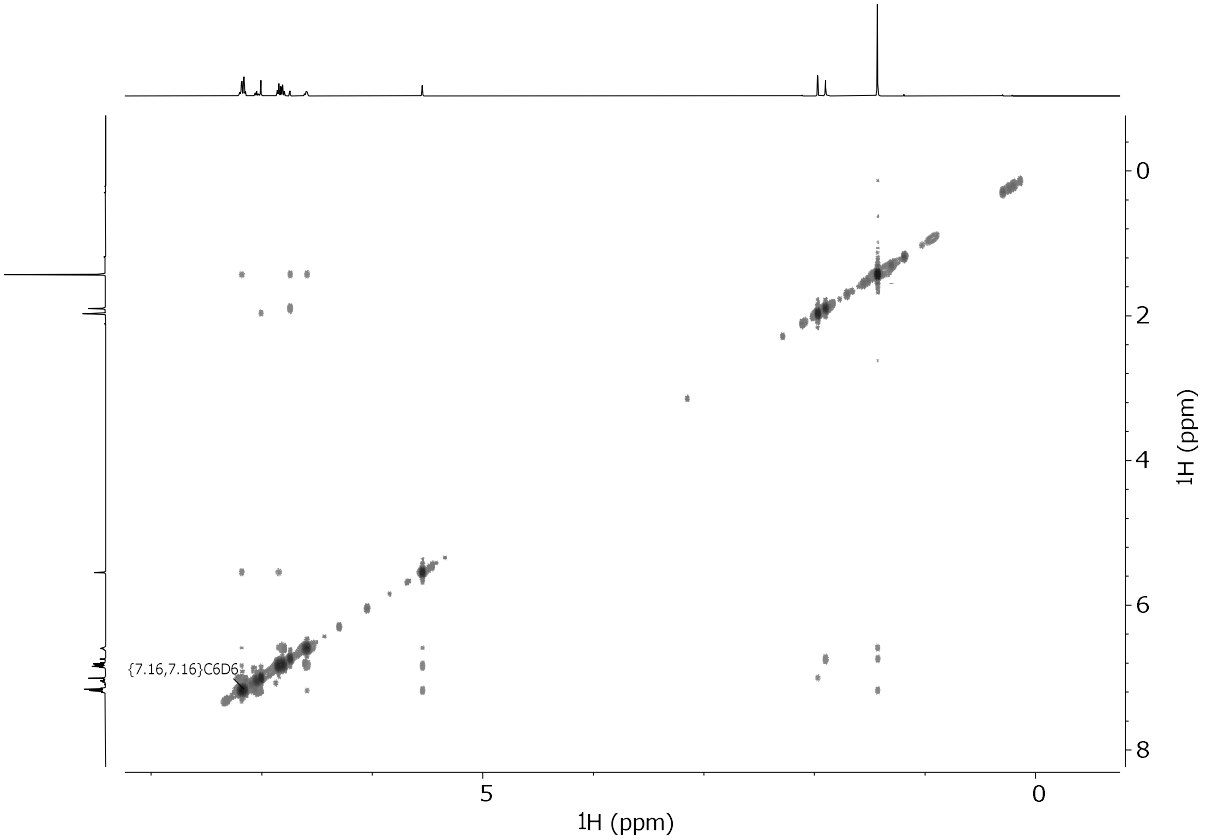


Figure S 48 *^{1}H-^{1}H NOESY NMR spectrum of ^{Ar*}NONK$_2$ in C_6D_6 at 298 K.*

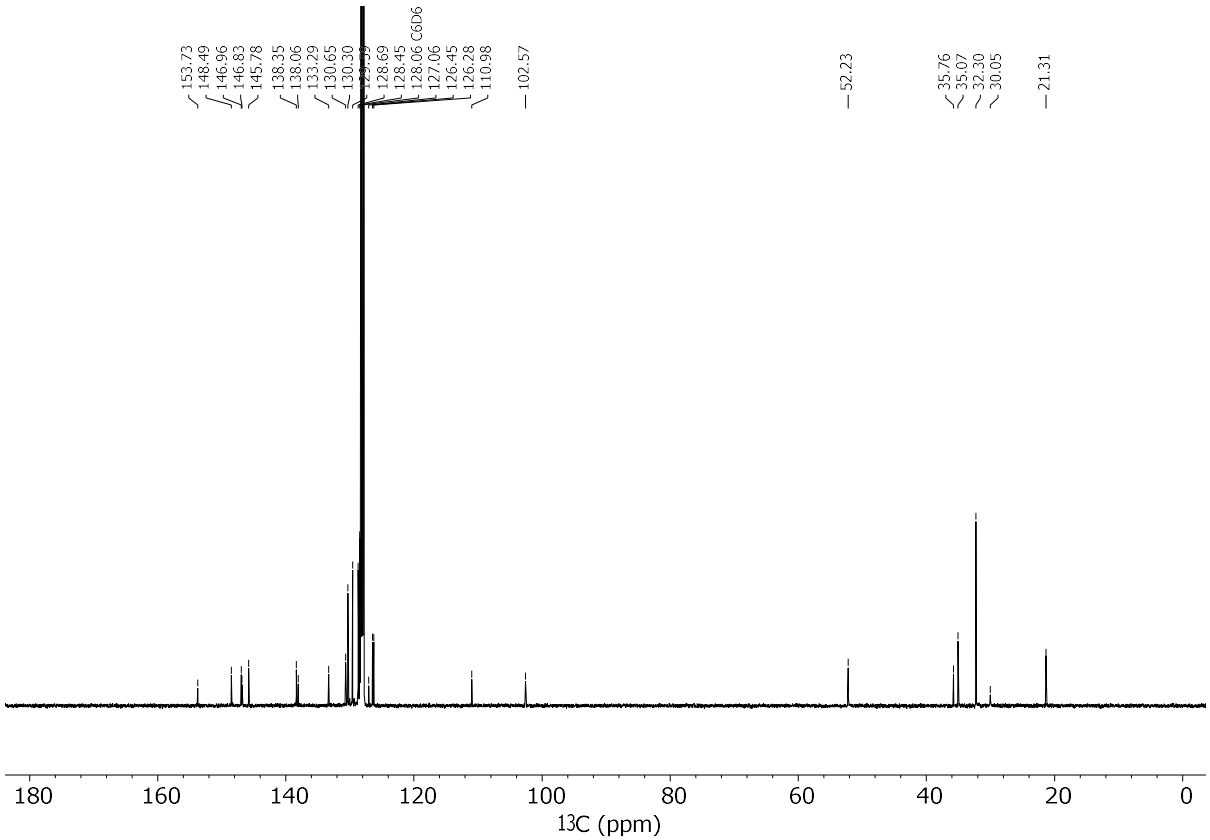


Figure S 49 *$^{13}C\{^1H\}$ NMR spectrum of $^{Ar*}NONK_2$ in C_6D_6 at 298 K.*

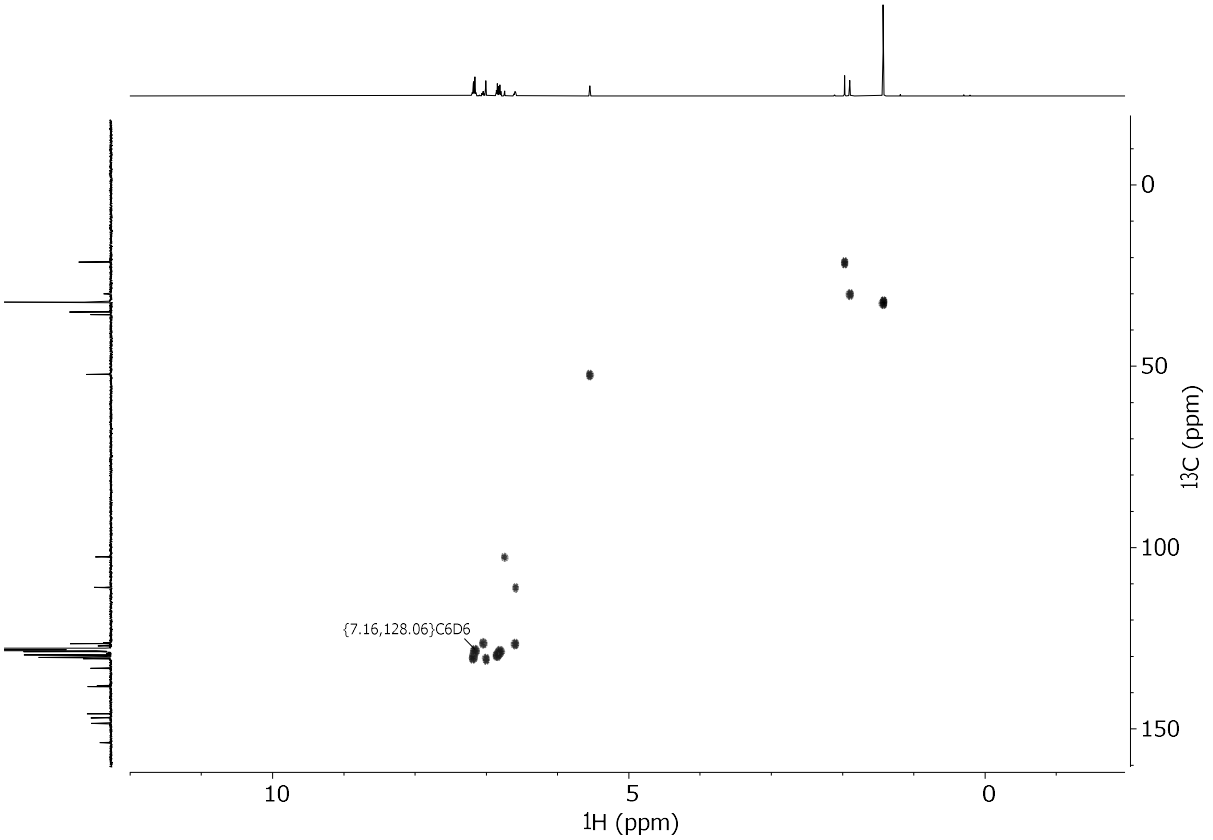


Figure S 50 *^{13}C-^{1}H HSQC NMR spectrum of $^{Ar^*}NONK_2$ in C_6D_6 at 298 K.*

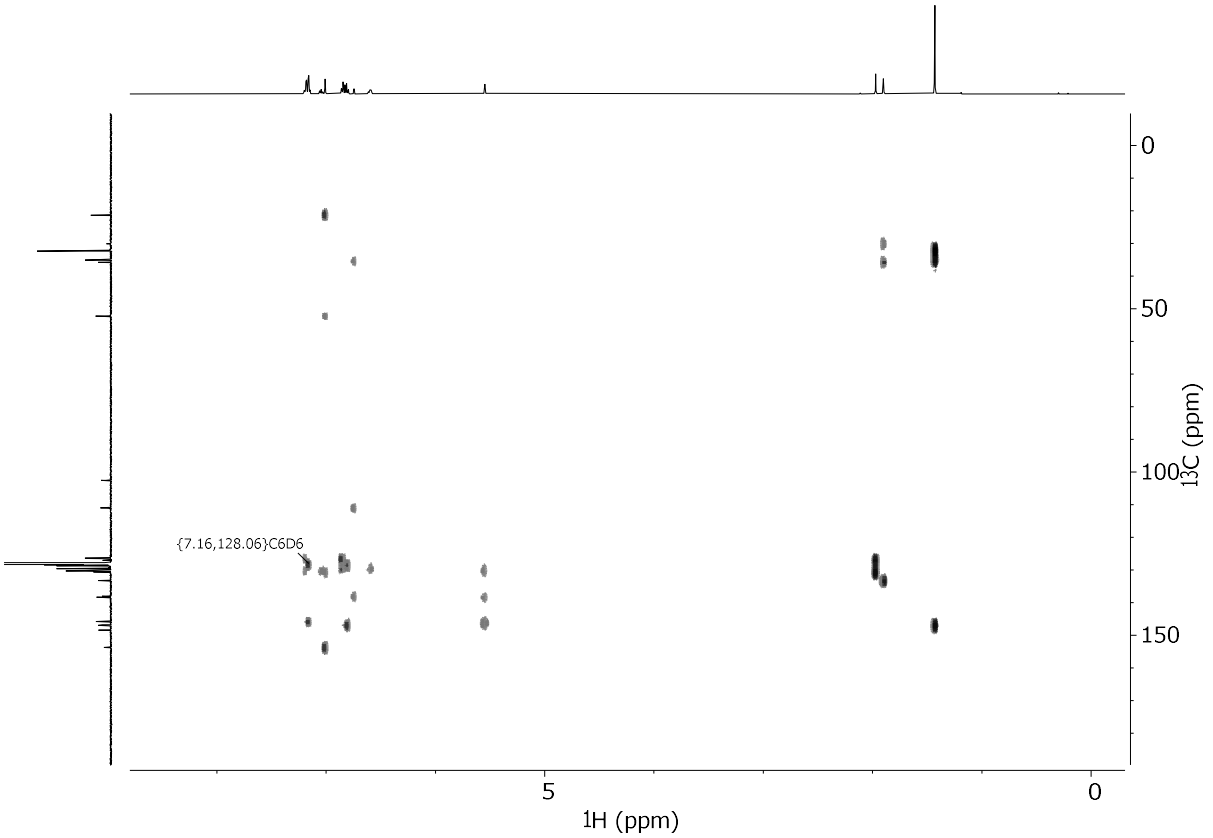


Figure S 51 *^{13}C-^{1}H HMBC NMR spectrum of $^{Ar*}NONK_2$ in C_6D_6 at 298 K.*

(^{Ar*}NON)Ca (1-□)

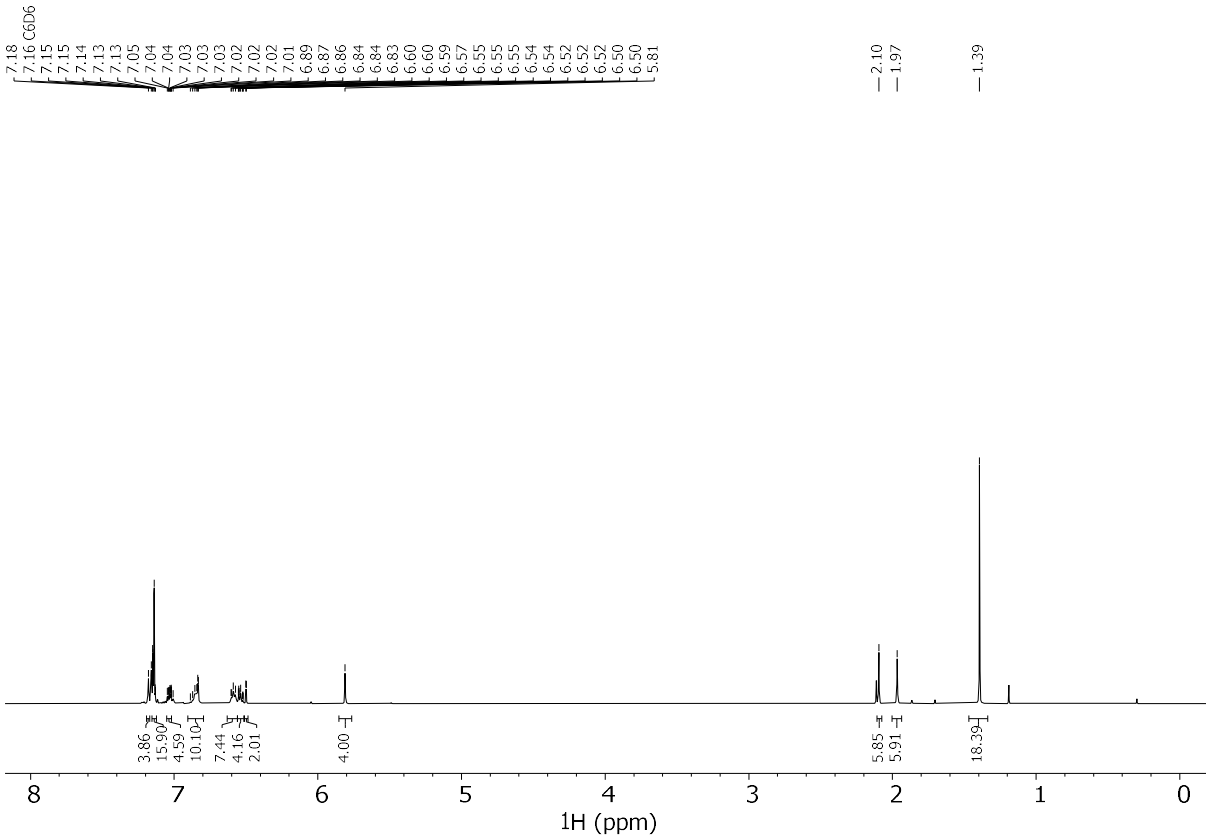


Figure S 52 *^{1}H NMR spectrum of **1**-□ in C_6D_6 at 298 K.*

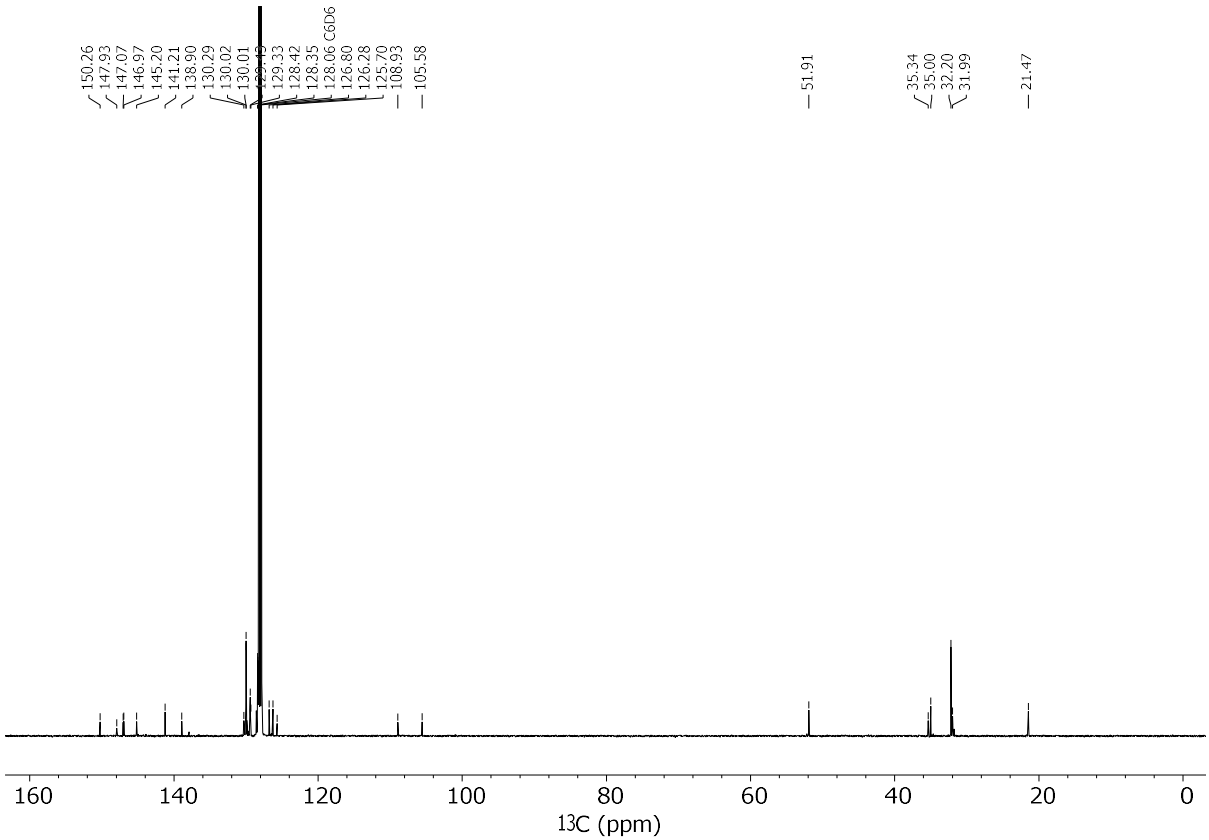


Figure S 53 *$^{13}C\{^{1}H\}$ NMR spectrum of **1**-□ in C_6D_6 at 298 K.*

(^{Ar*}NON)Ca(thf) (1-thf)

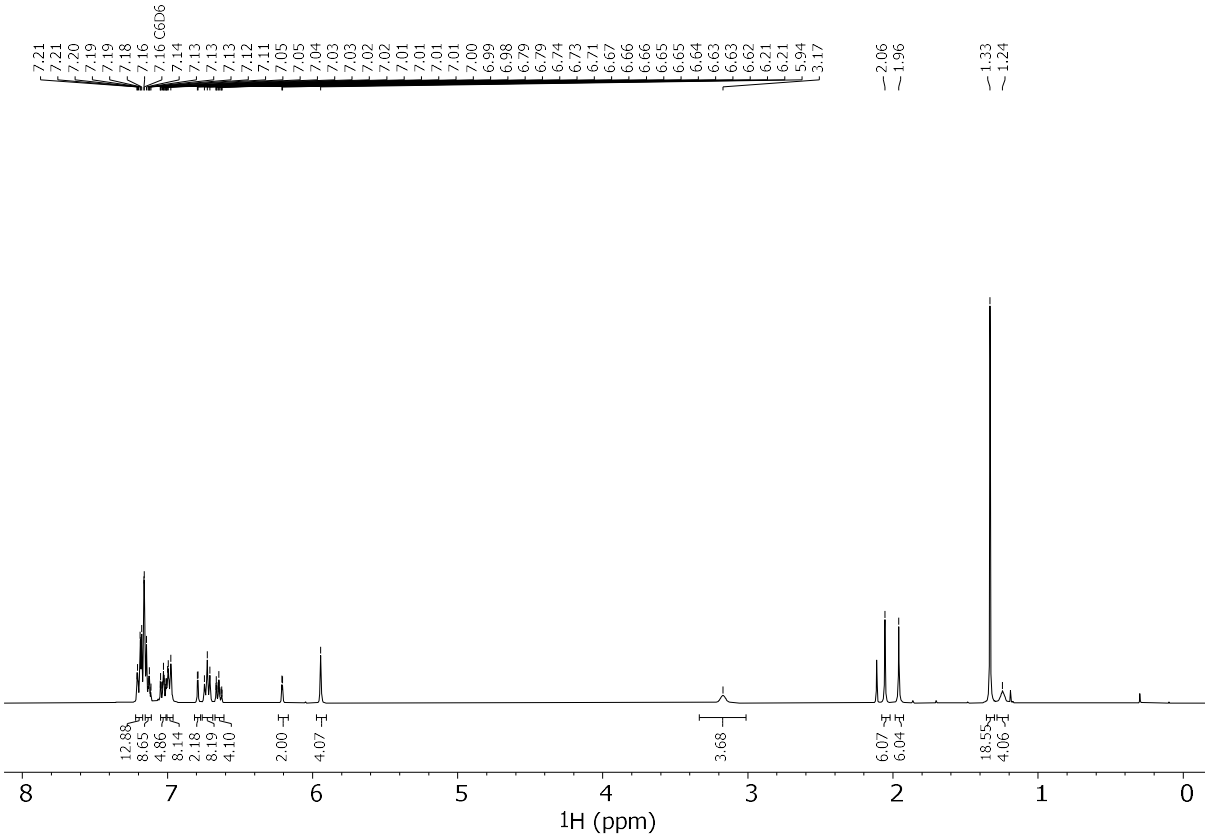


Figure S 54 *^{1}H NMR spectrum of **1**-thf in C_6D_6 at 298 K.*

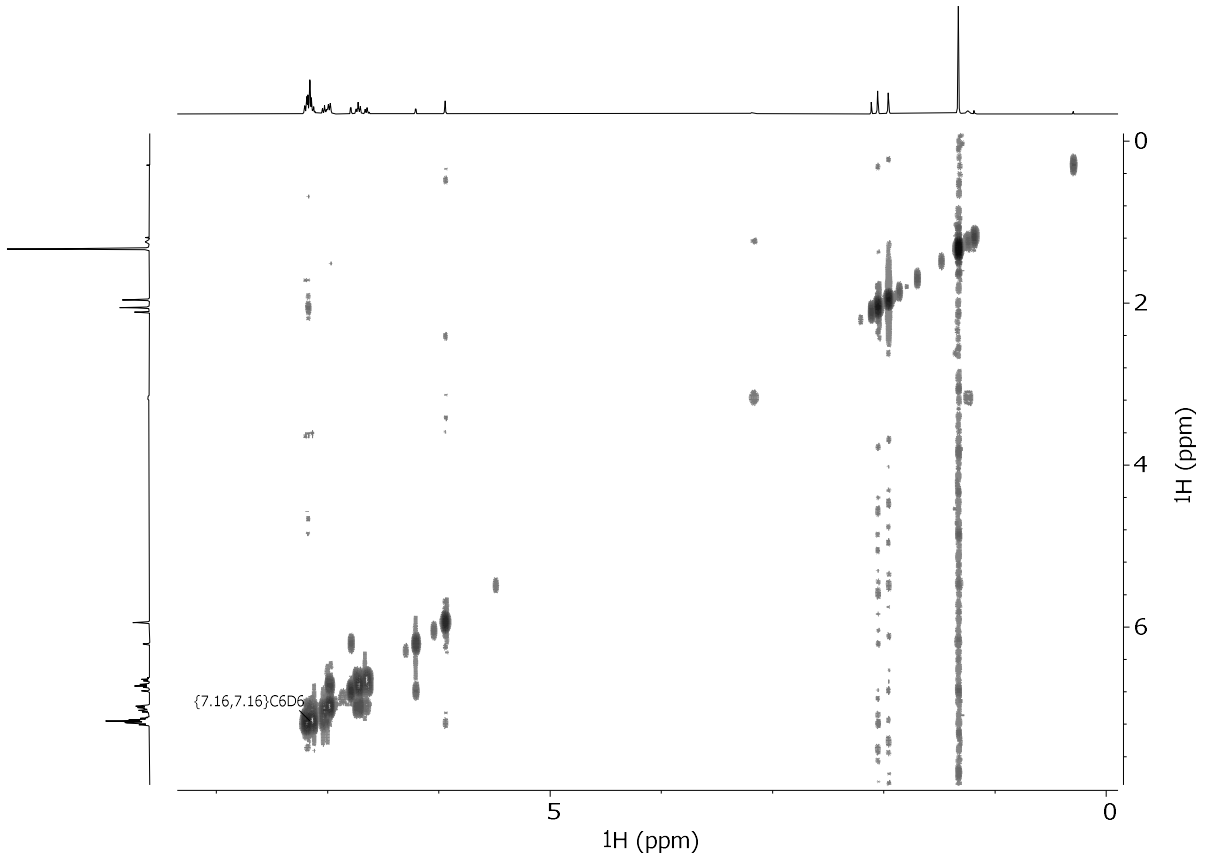


Figure S 55 *^{1}H-^{1}H COSY NMR spectrum of **1**-thf in C_6D_6 at 298 K.*

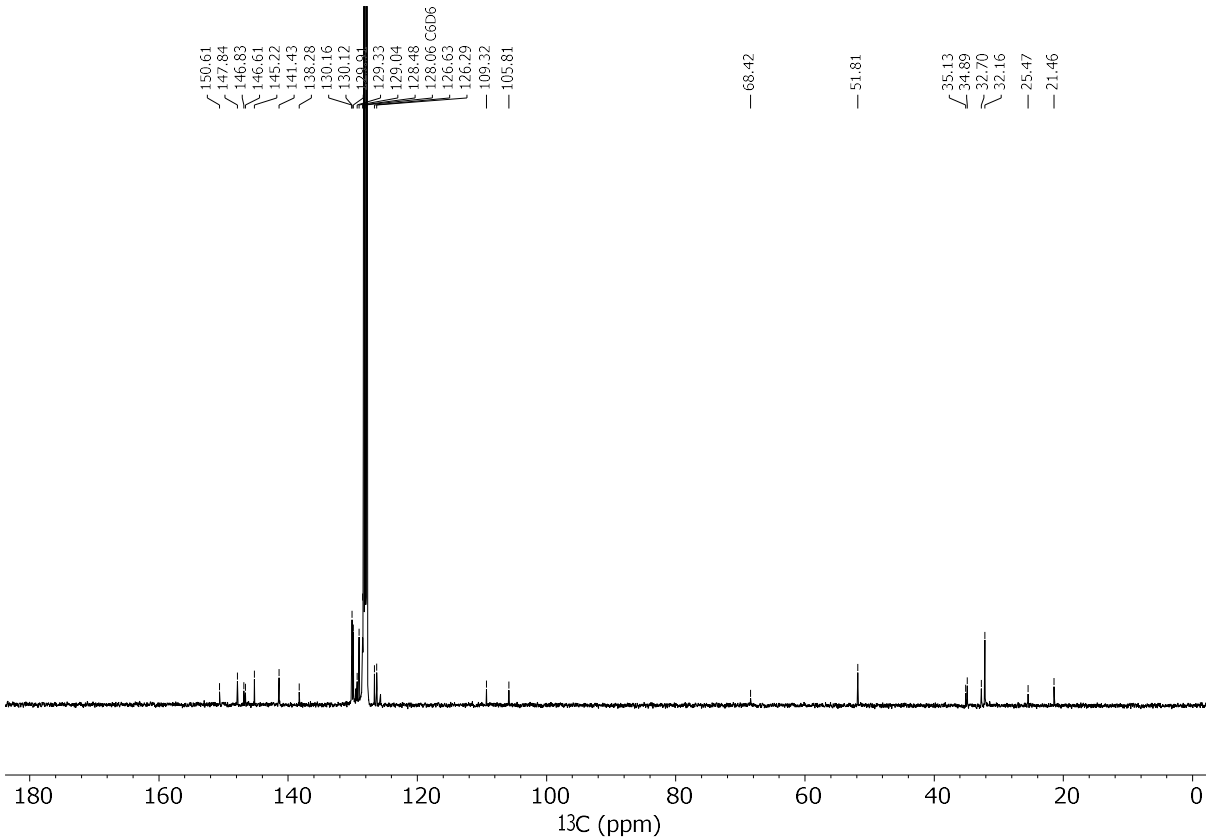


Figure S 56 *$^{13}C\{^{1}H\}$ NMR spectrum of **1**-thf in C_6D_6 at 298 K.*

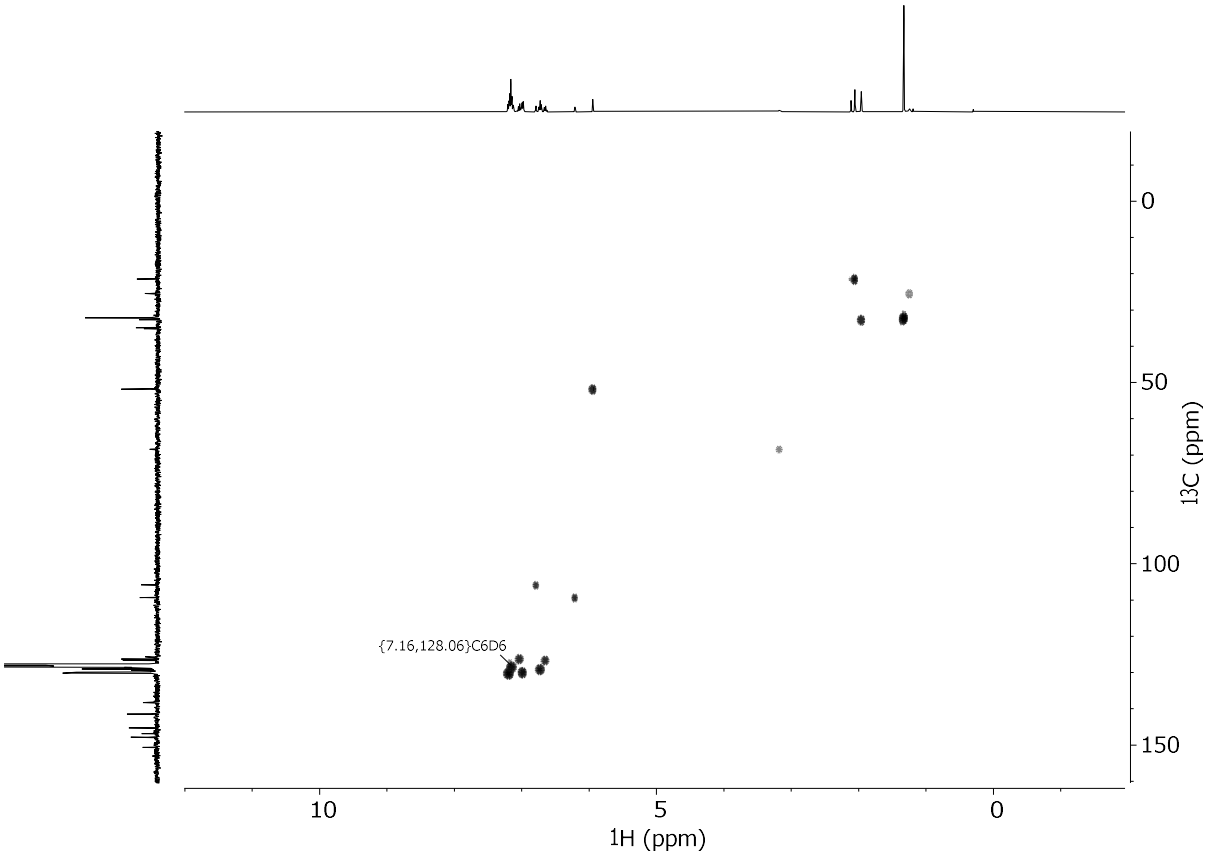


Figure S 57 *^{13}C-^{1}H HSQC NMR spectrum of **1**-thf in C_6D_6 at 298 K.*

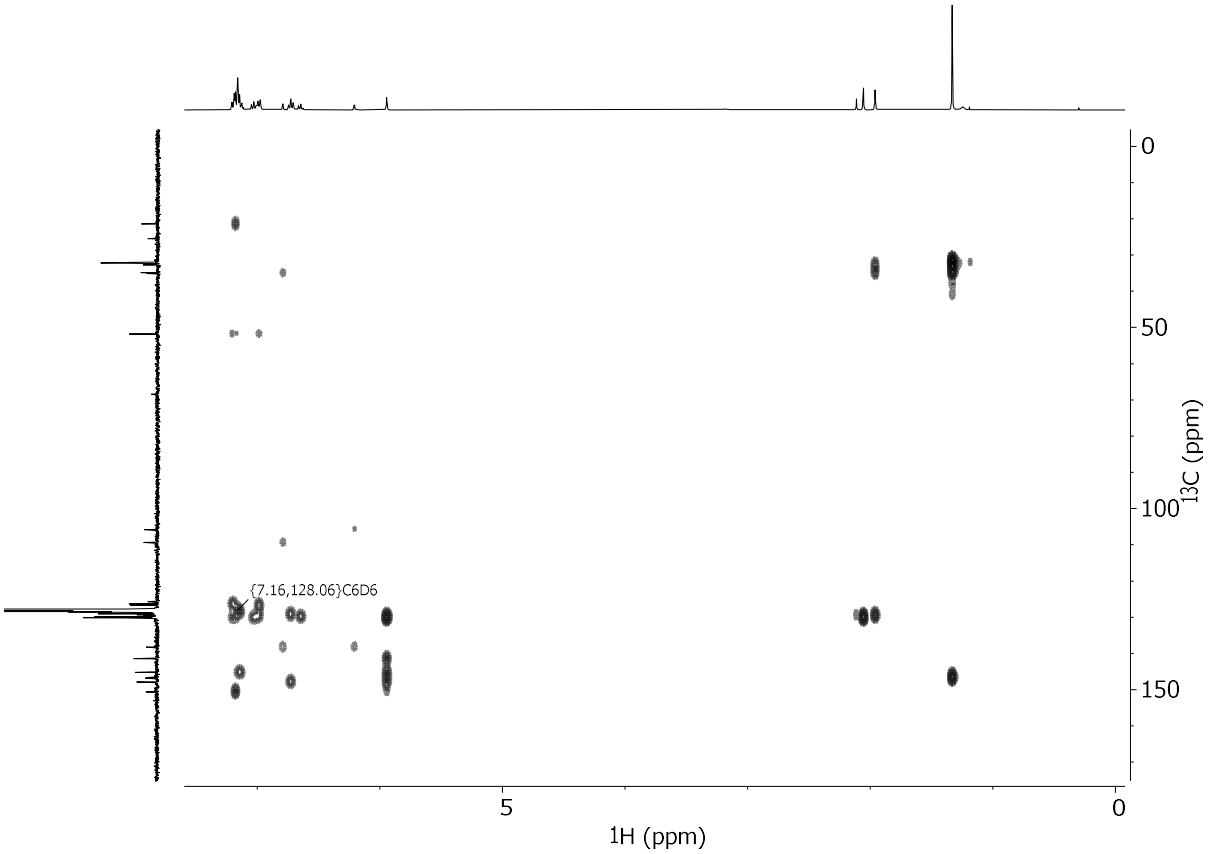


Figure S 58 *^{13}C-^{1}H HMBC NMR spectrum of **1**-thf in C_6D_6 at 298 K.*

(^{Ar*}NON)Ca (1-□)

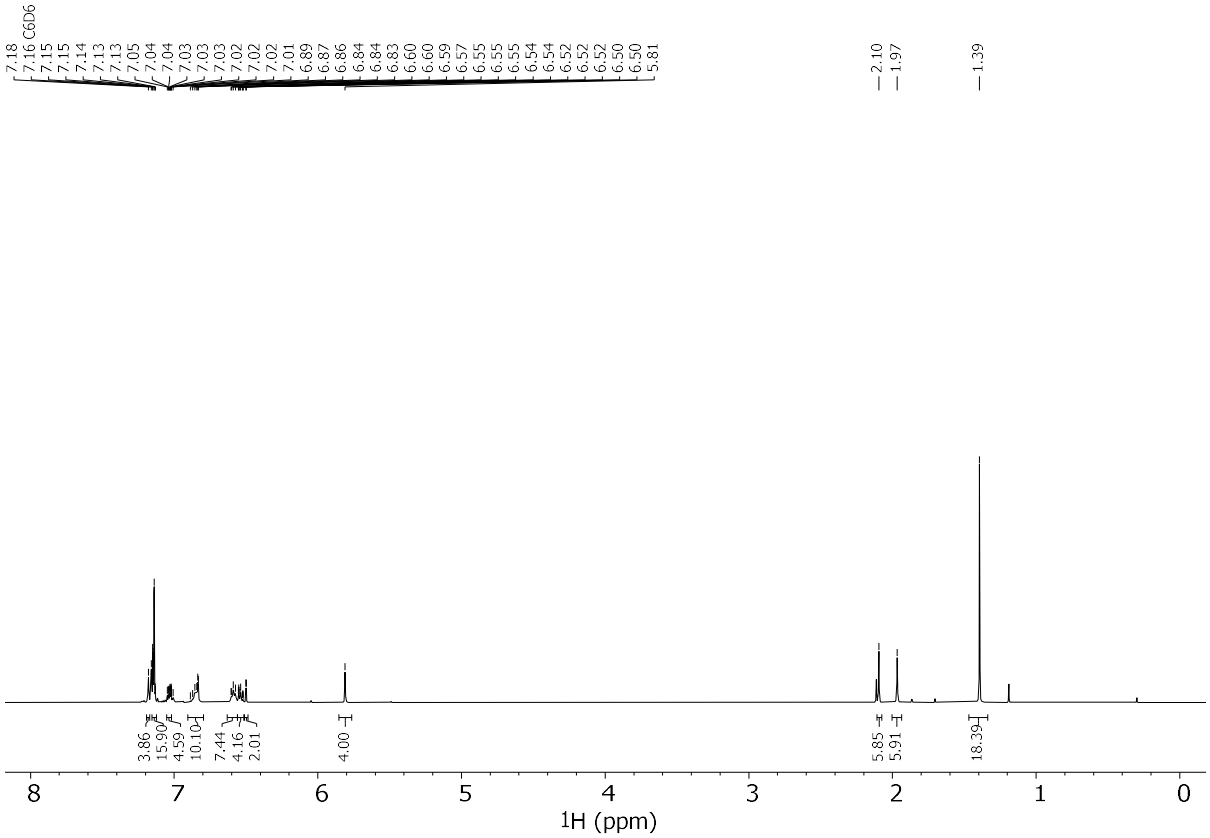


Figure S 59 *^{1}H NMR spectrum of 1-□ in C_6D_6 at 298 K.*

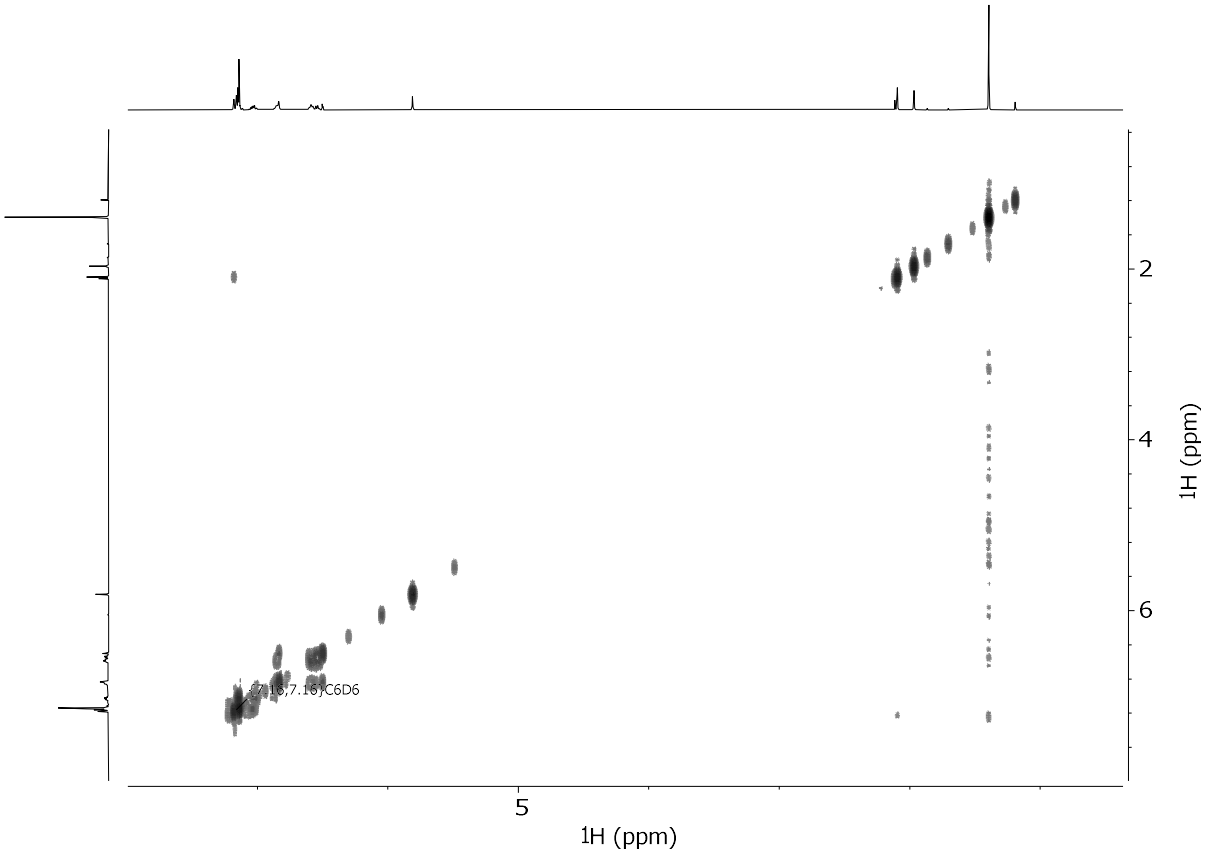


Figure S 60 *^{1}H-^{1}H COSY NMR spectrum of 1-□ in C_6D_6 at 298 K.*

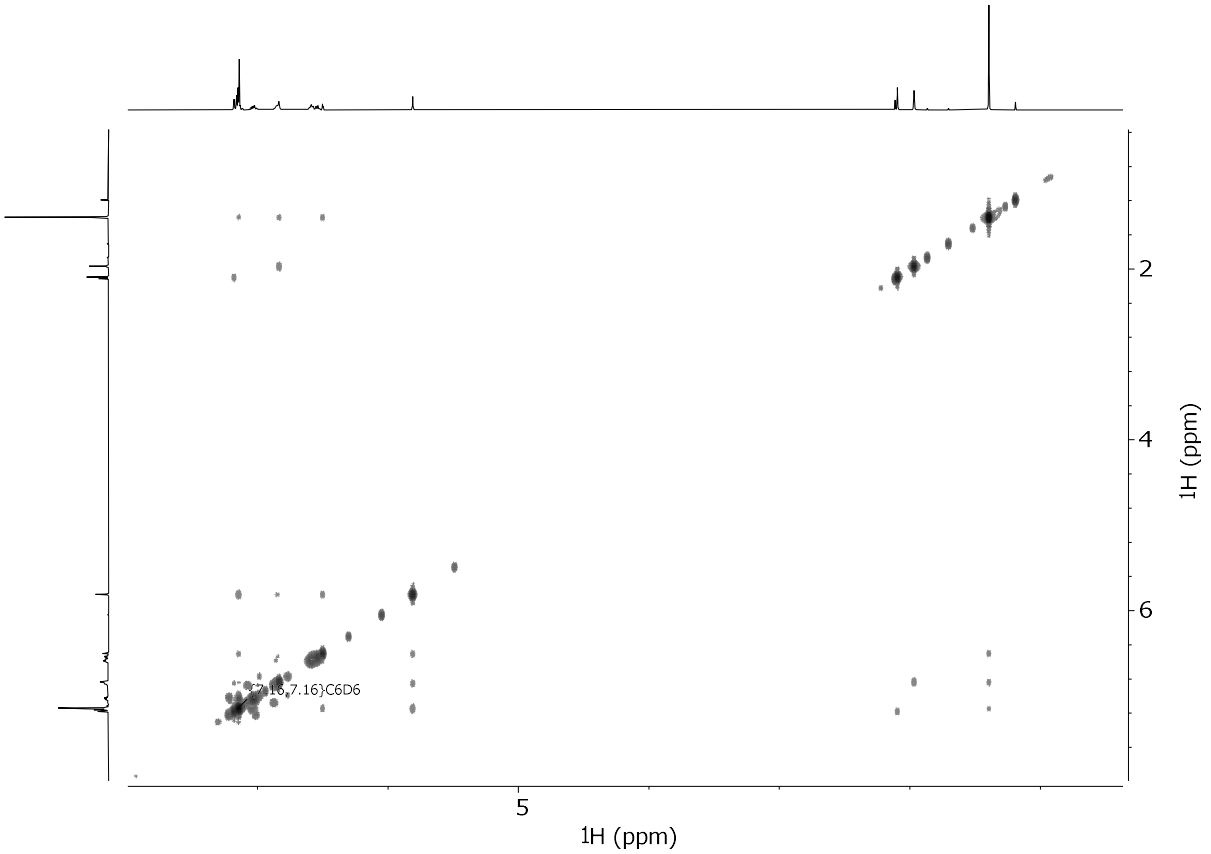


Figure S 61 *^{1}H-^{1}H ROESY NMR spectrum of 1-□ in C_6D_6 at 298 K.*

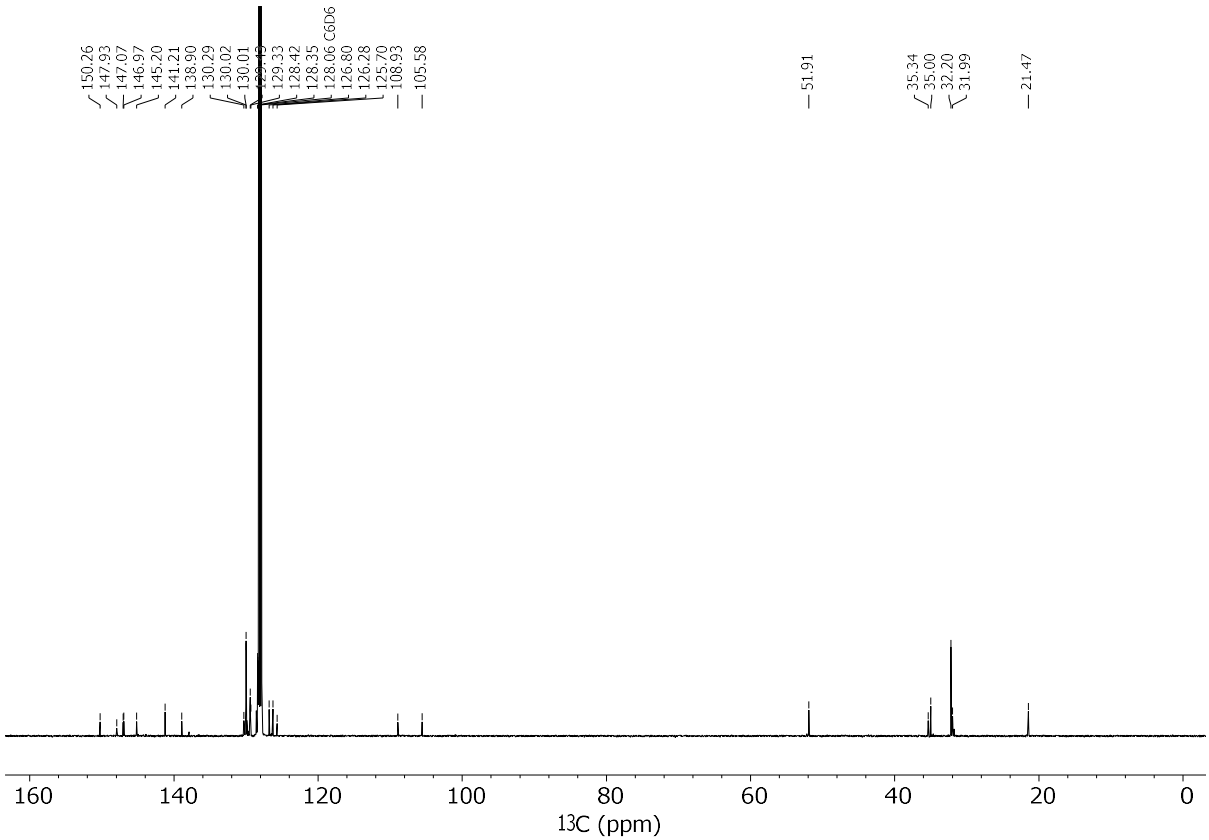


Figure S 62 *$^{13}C\{^{1}H\}$ NMR spectrum of 1-□ in C_6D_6 at 298 K.*

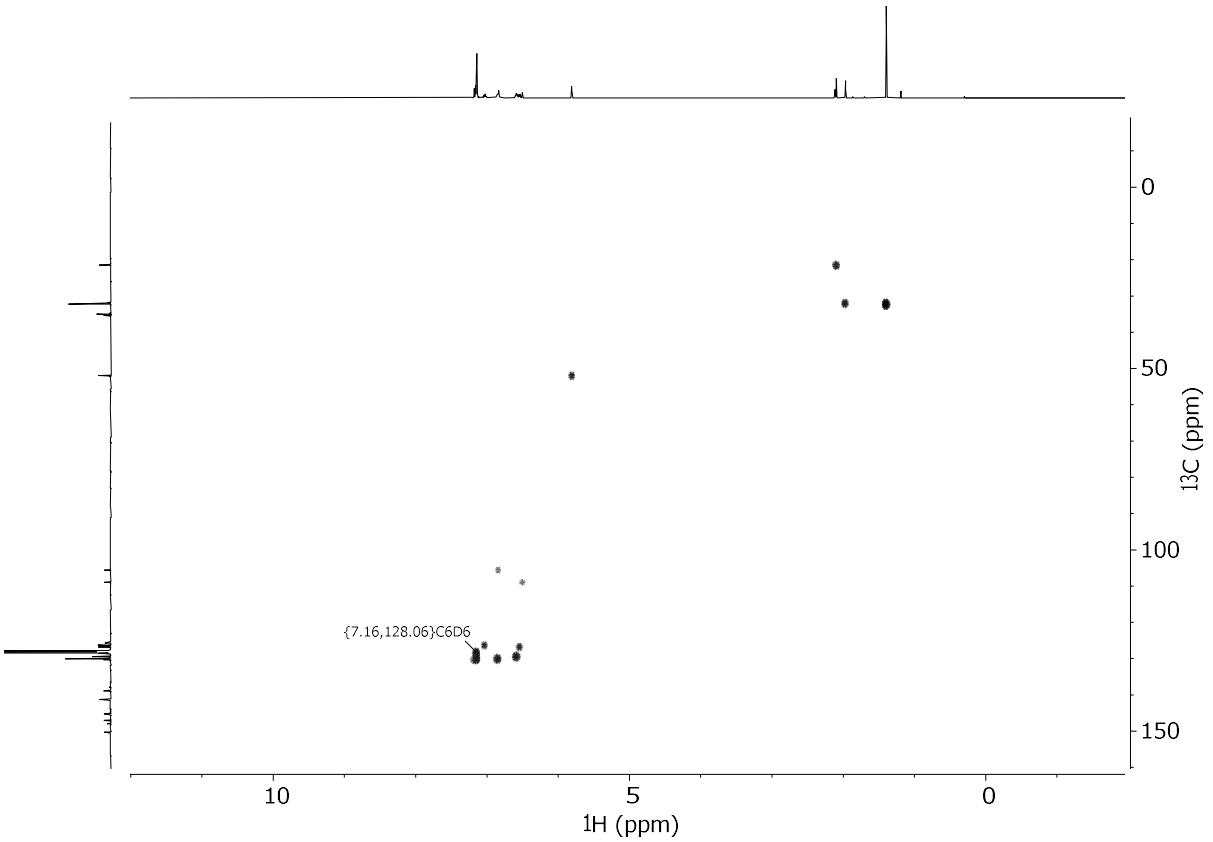


Figure S 63 *^{13}C-^{1}H HSQC NMR spectrum of 1-□ in C_6D_6 at 298 K.*

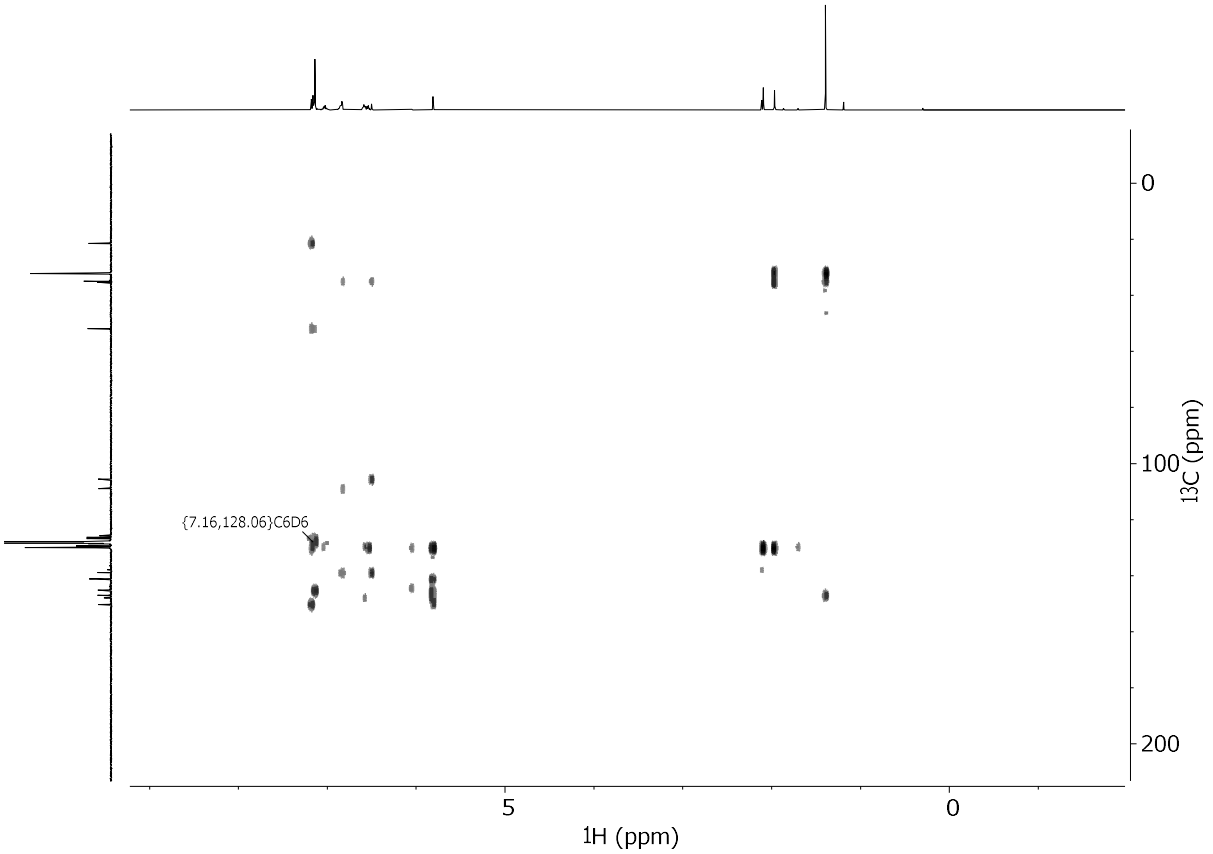


Figure S 64 *^{13}C-^{1}H HMBC NMR spectrum of 1-□ in C_6D_6 at 298 K.*

(^{Ar*}NON)Mg(thf)(tol)

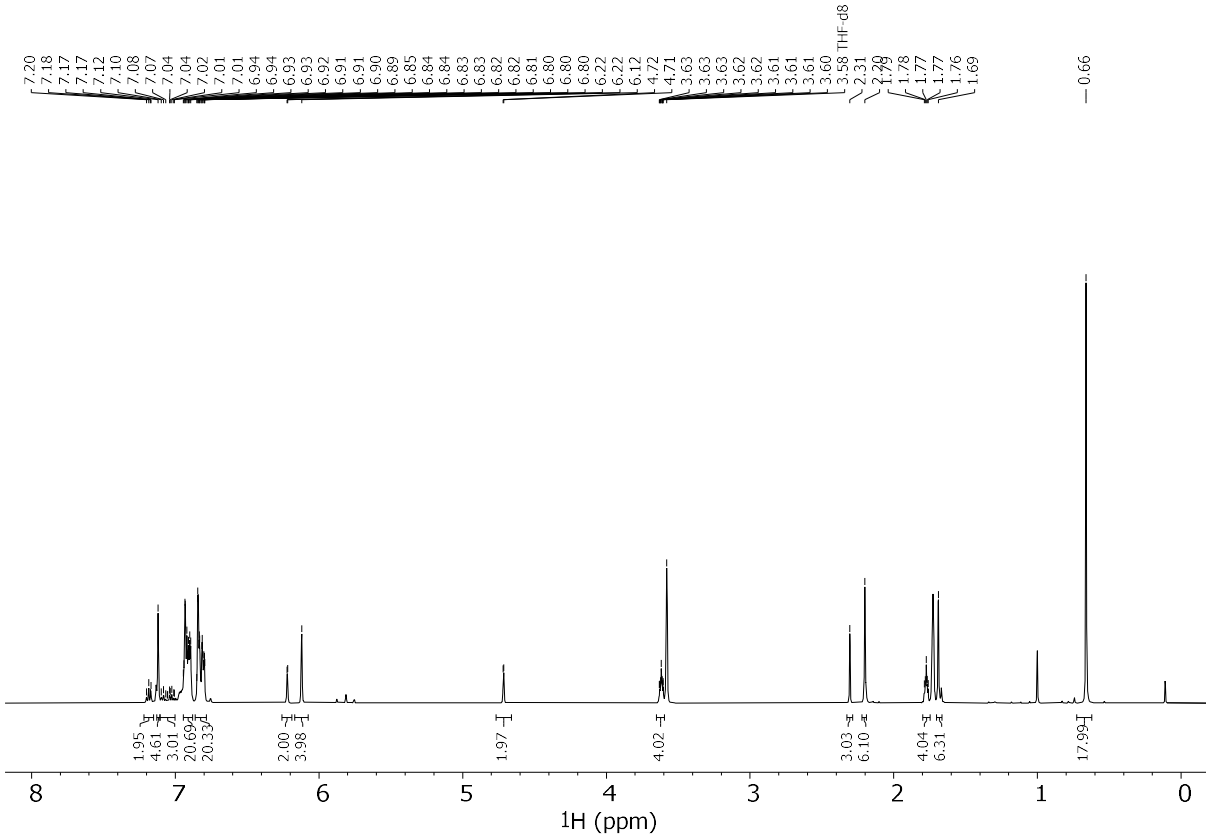


Figure S 65 *^{1}H NMR spectrum of (^{Ar*}NON)Mg(thf)(tol) in thf-d_8 at 298 K.*

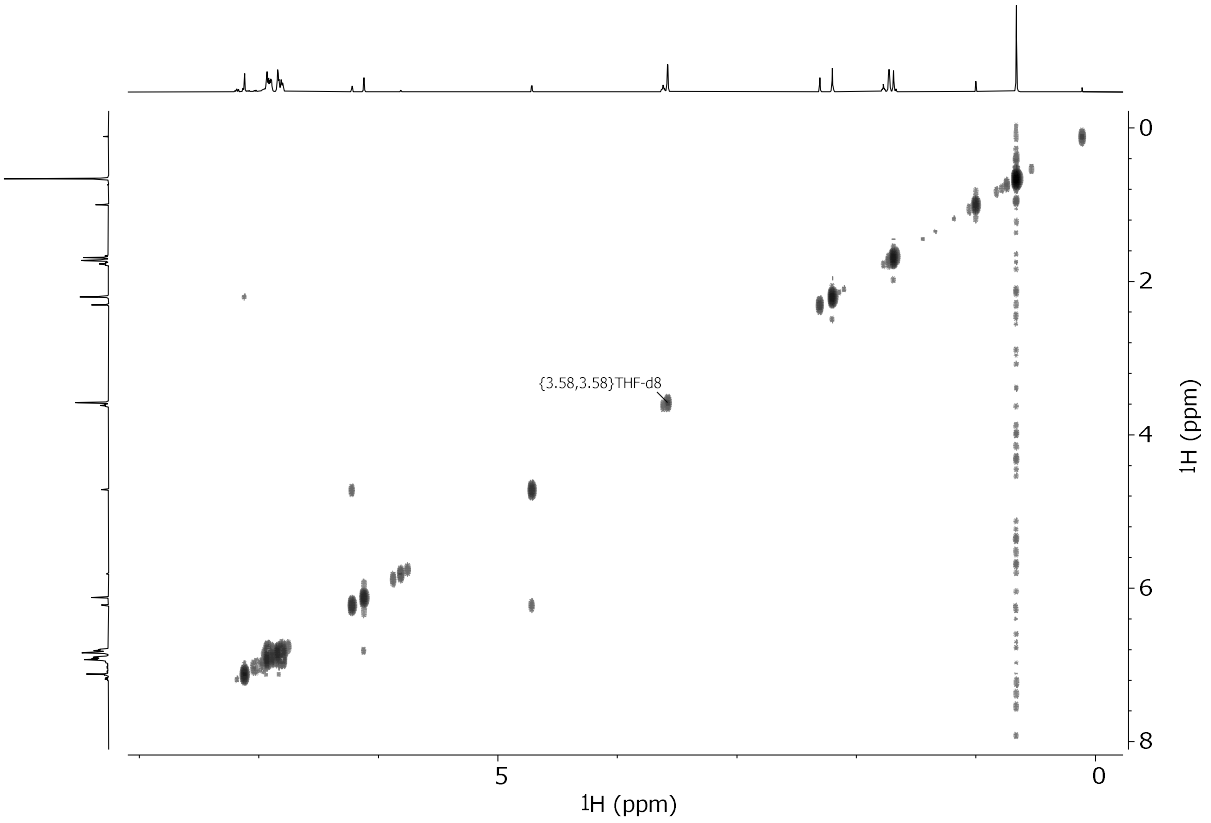


Figure S 66 *^{1}H-^{1}H COSY NMR spectrum of (^{Ar*}NON)Mg(thf)(tol) in thf-d_8 at 298 K.*

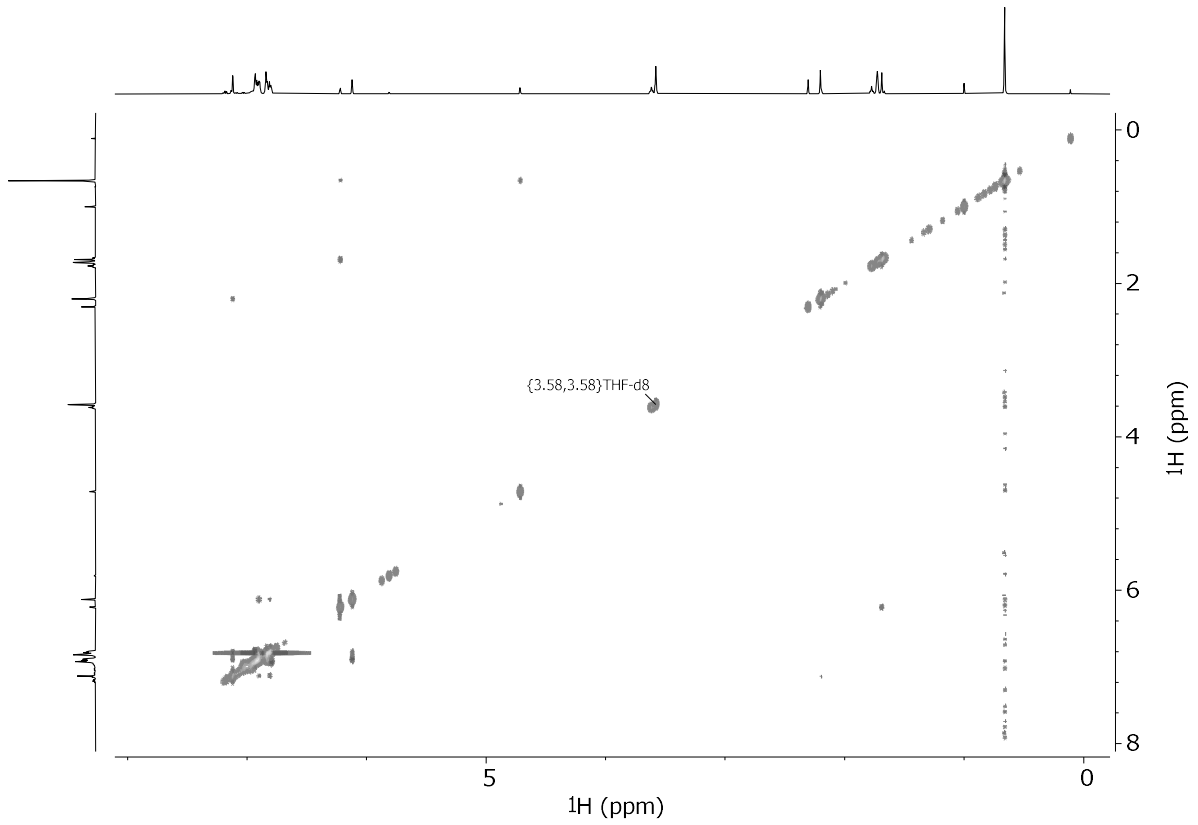


Figure S 67 *^{1}H-^{1}H ROESY NMR spectrum of (^{Ar*}NON)Mg(thf)(tol) in thf-d_8 at 298 K.*

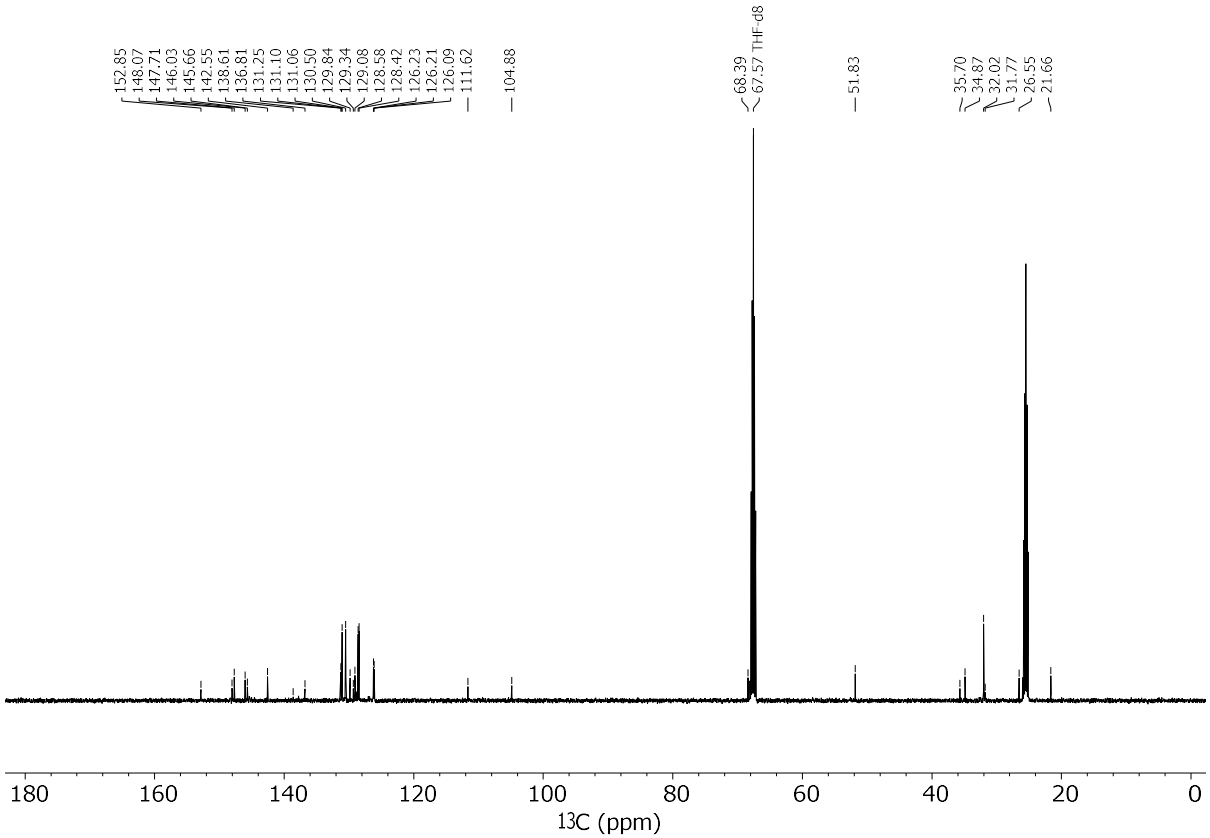


Figure S 68 *$^{13}C\{^{1}H\}$ NMR spectrum of (^{Ar*}NON)Mg(thf)(tol) in thf-d_8 at 298 K.*

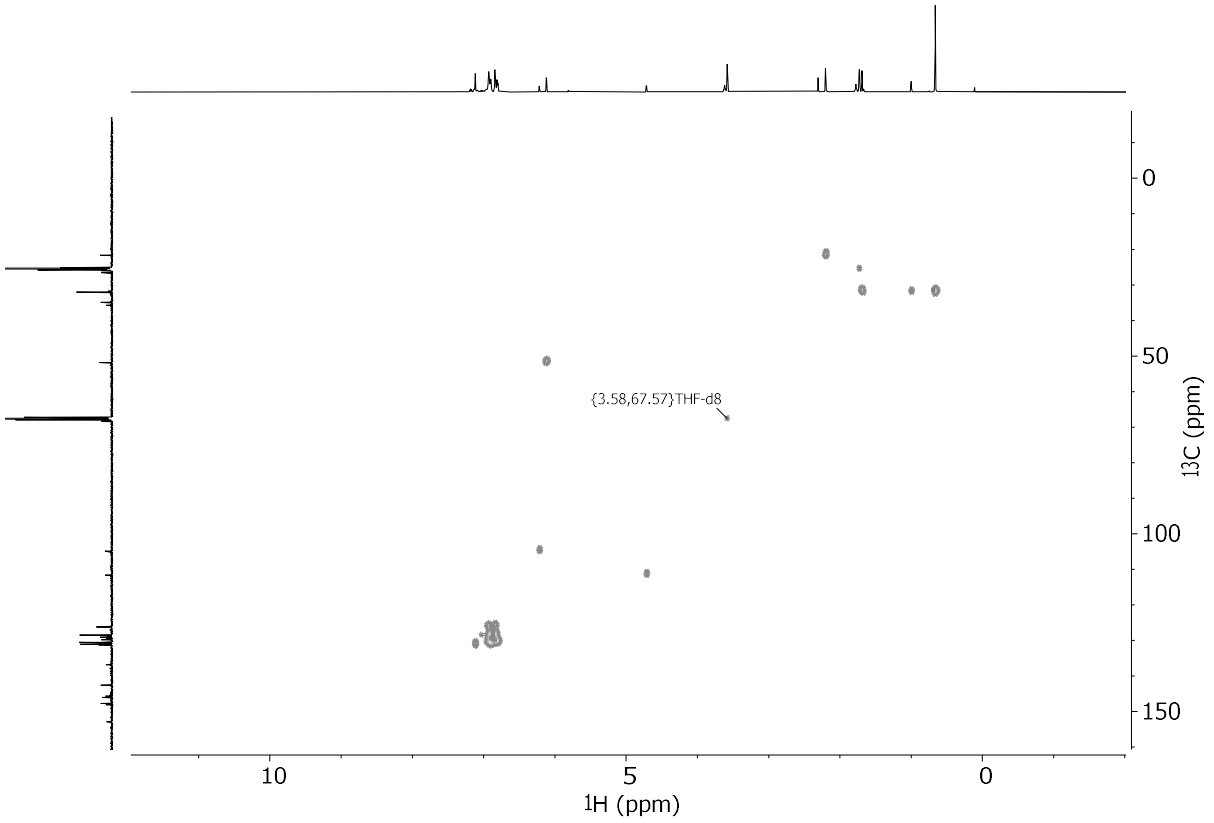


Figure S 69 *^{13}C-^{1}H HSQC NMR spectrum of (^{Ar*}NON)Mg(thf)(tol) in thf-d_8 at 298 K.*

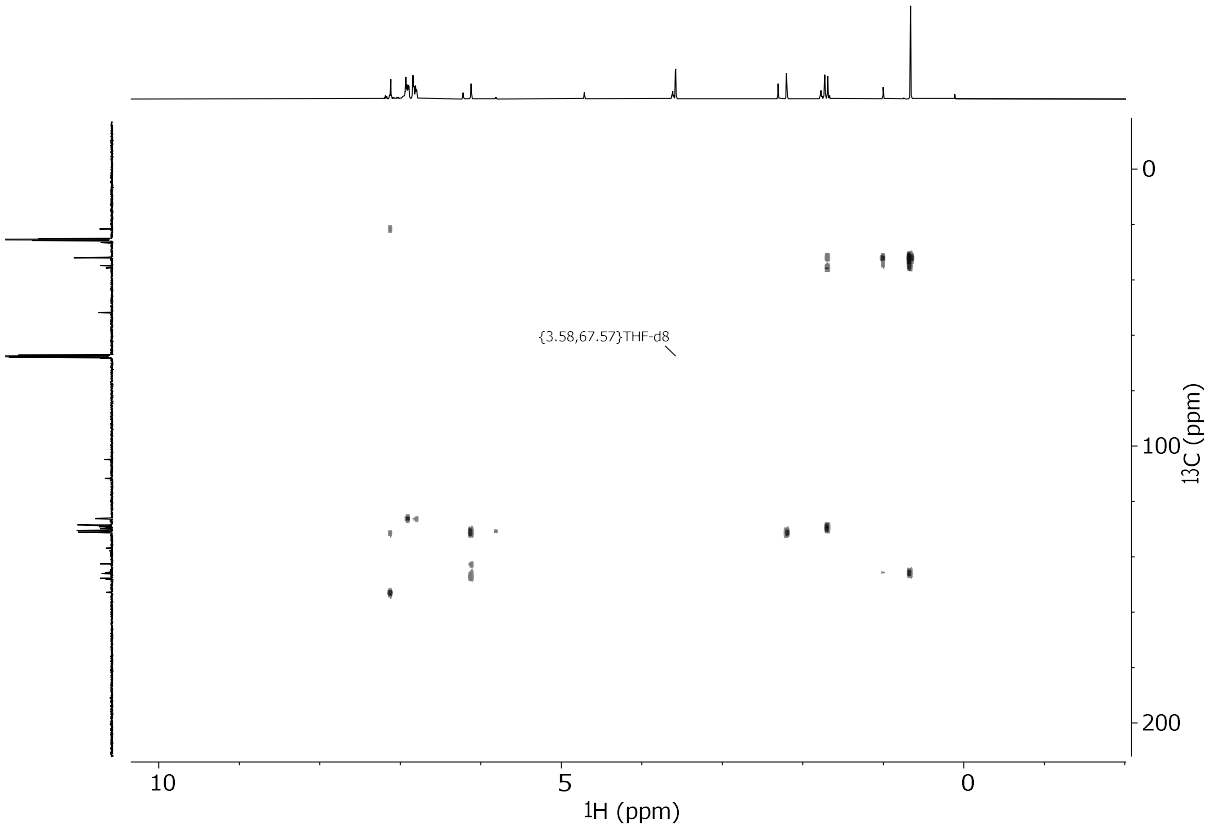


Figure S 70 *^{13}C-^{1}H HMBC NMR spectrum of (^{Ar*}NON)Mg(thf)(tol) in thf-d_8 at 298 K.*

(^{Ar*}NON)Sr

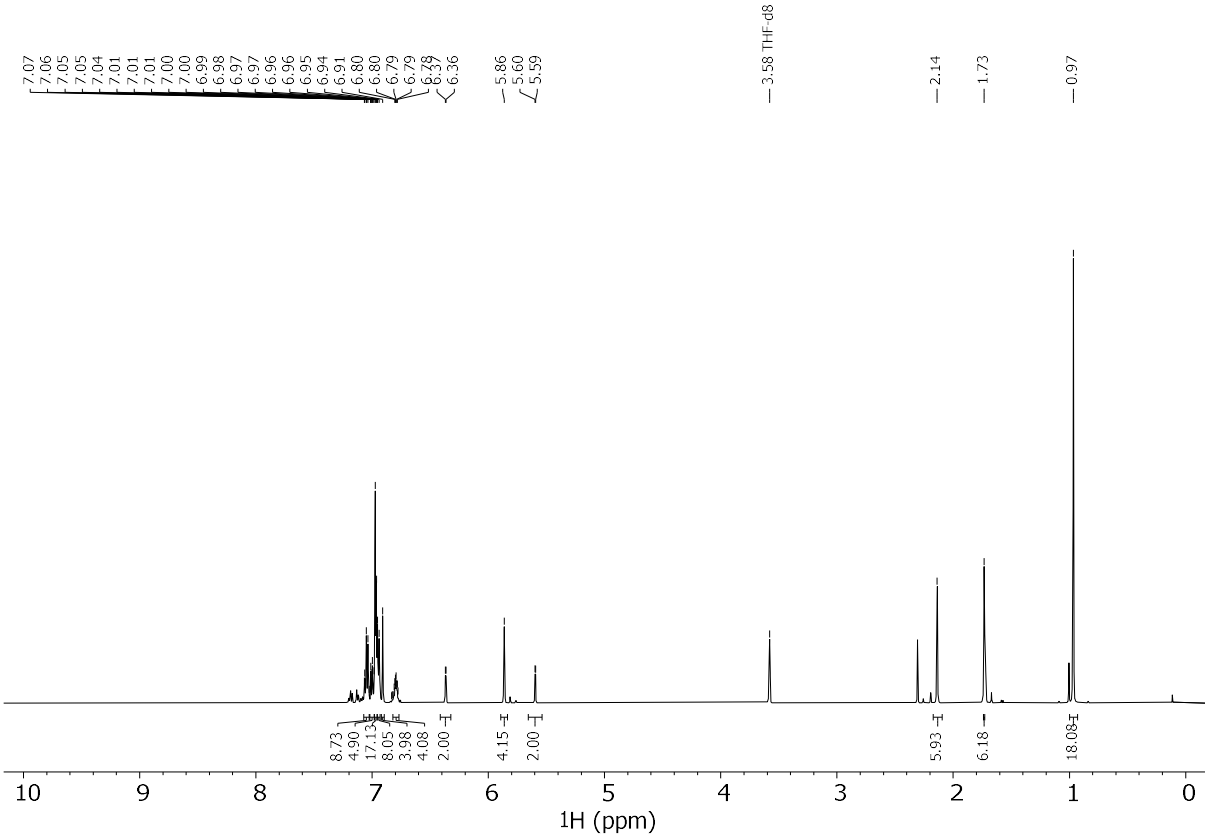


Figure S 71 *^{1}H NMR spectrum of (^{Ar*}NON)Sr in thf-d_8 at 298 K.*

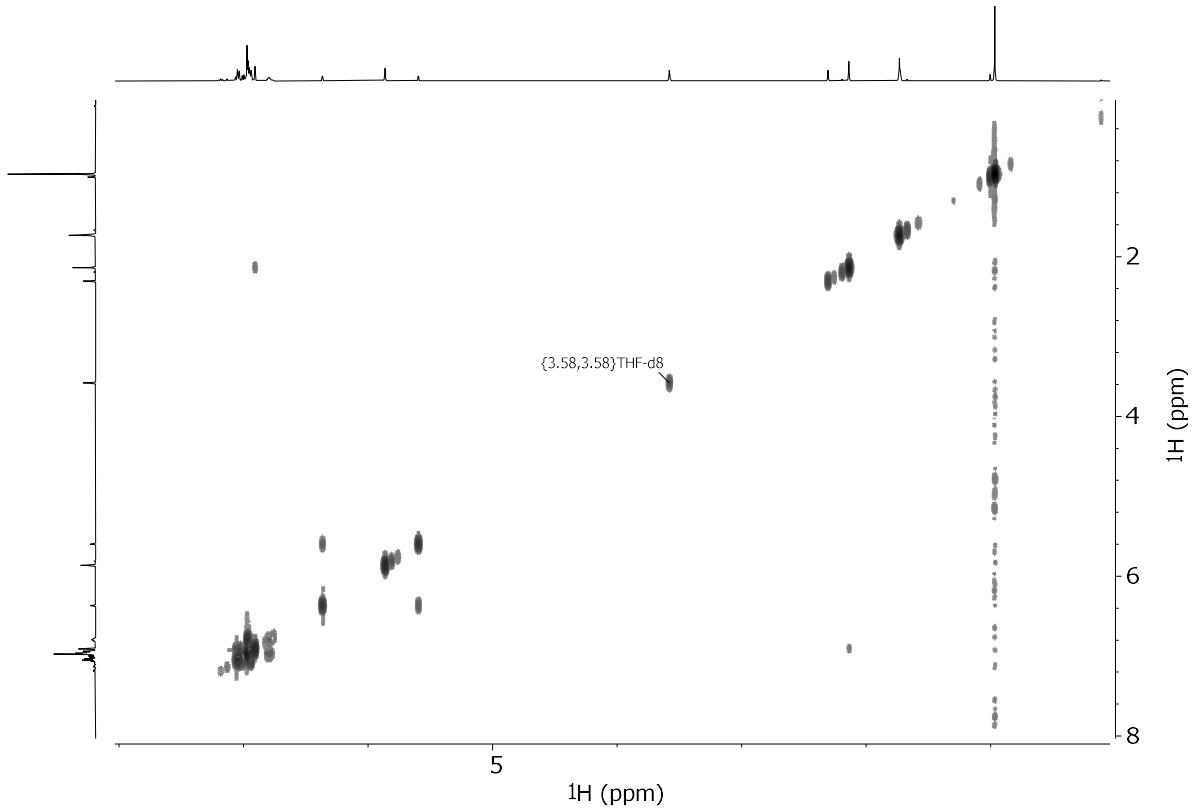


Figure S 72 *^{1}H-^{1}H COSY NMR spectrum of (^{Ar*}NON)Sr in thf-d_8 at 298 K.*

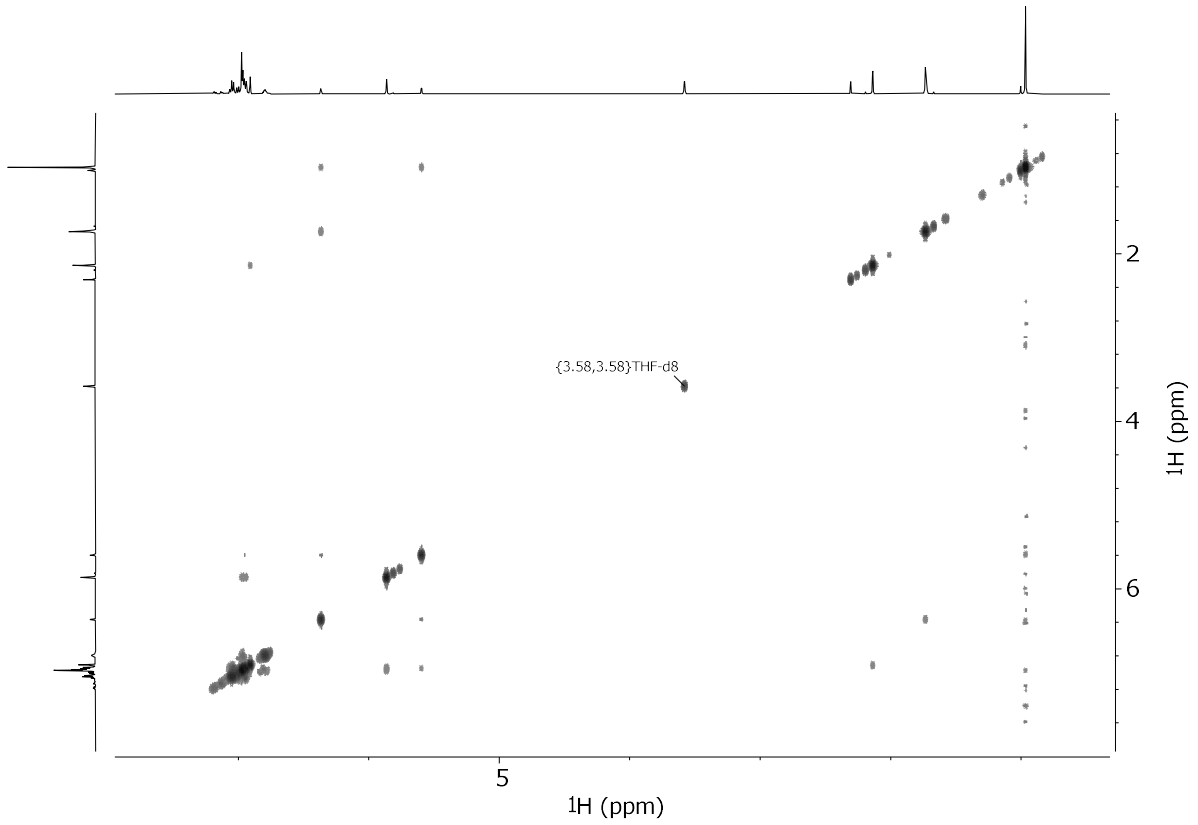


Figure S 73 *^{1}H-^{1}H NOESY NMR spectrum of (^{Ar*}NON)Sr in thf-d_8 at 298 K.*

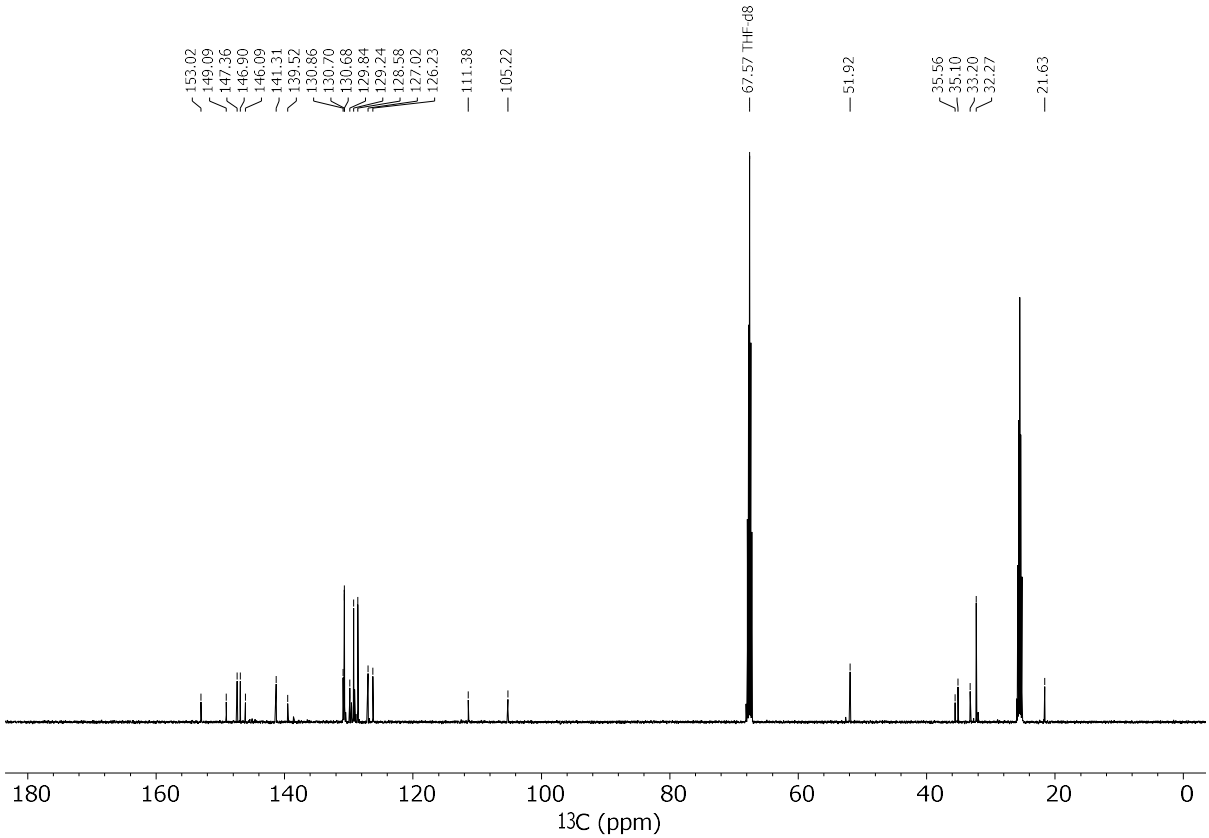


Figure S 74 *$^{13}C\{^{1}H\}$ NMR spectrum of (^{Ar*}NON)Sr in thf-d_8 at 298 K.*

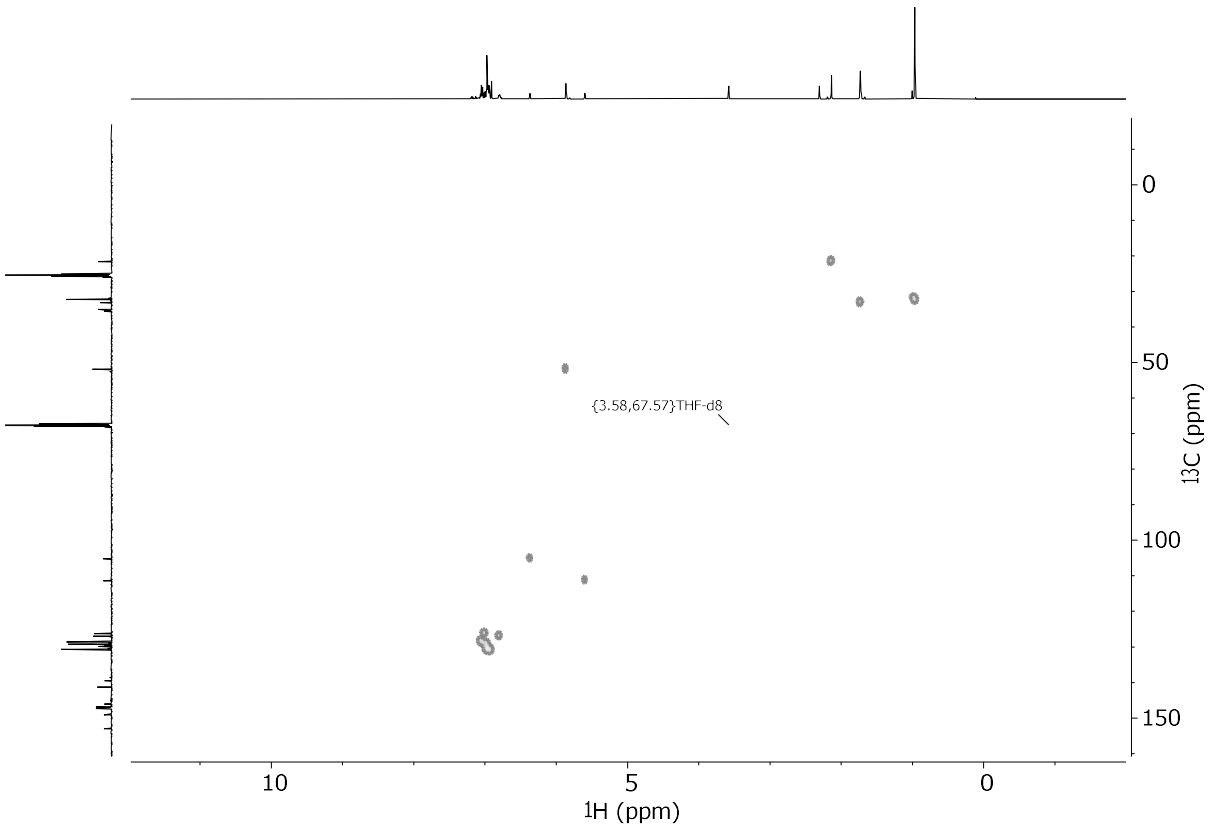


Figure S 75 *^{13}C-^{1}H HSQC NMR spectrum of (^{Ar*}NON)Sr in thf-d_8 at 298 K.*

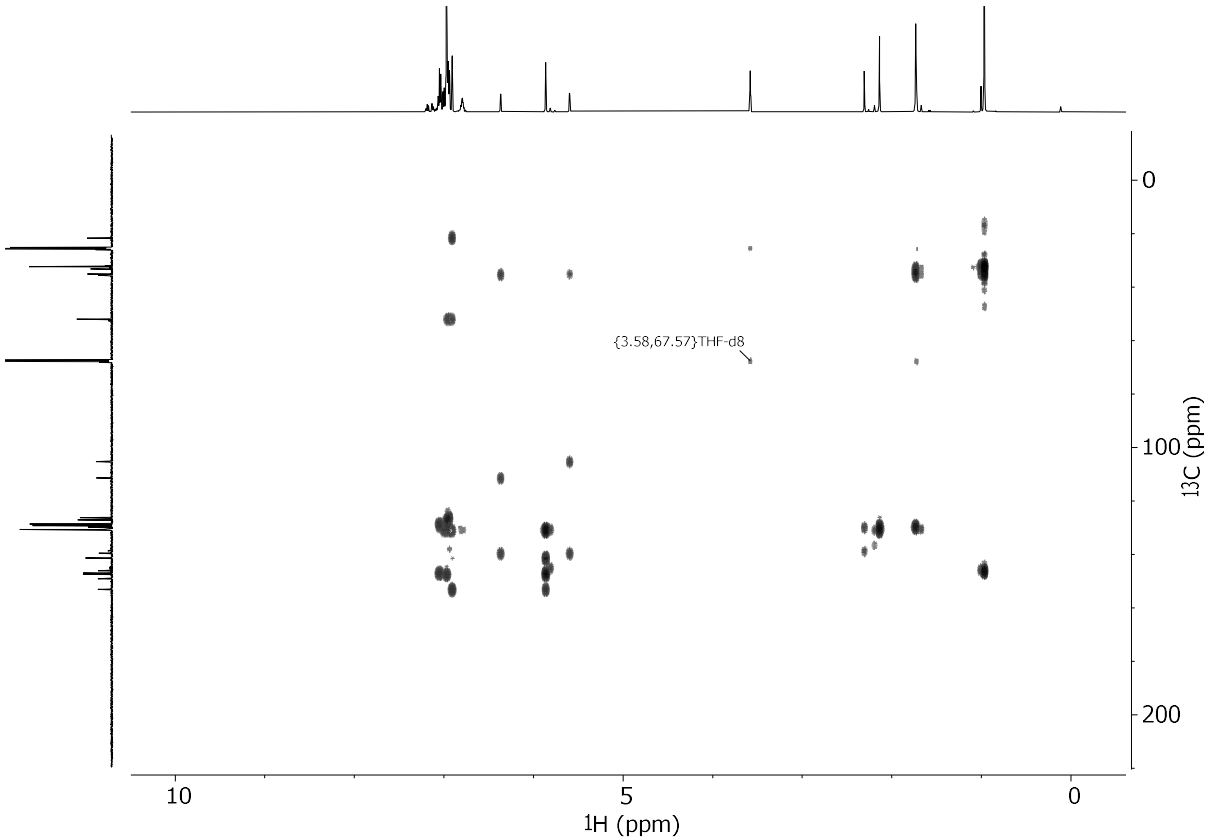


Figure S 76 *^{13}C-^{1}H HMBC NMR spectrum of (^{Ar*}NON)Sr in thf-d_8 at 298 K.*

(^{Ar*}NON)Ba

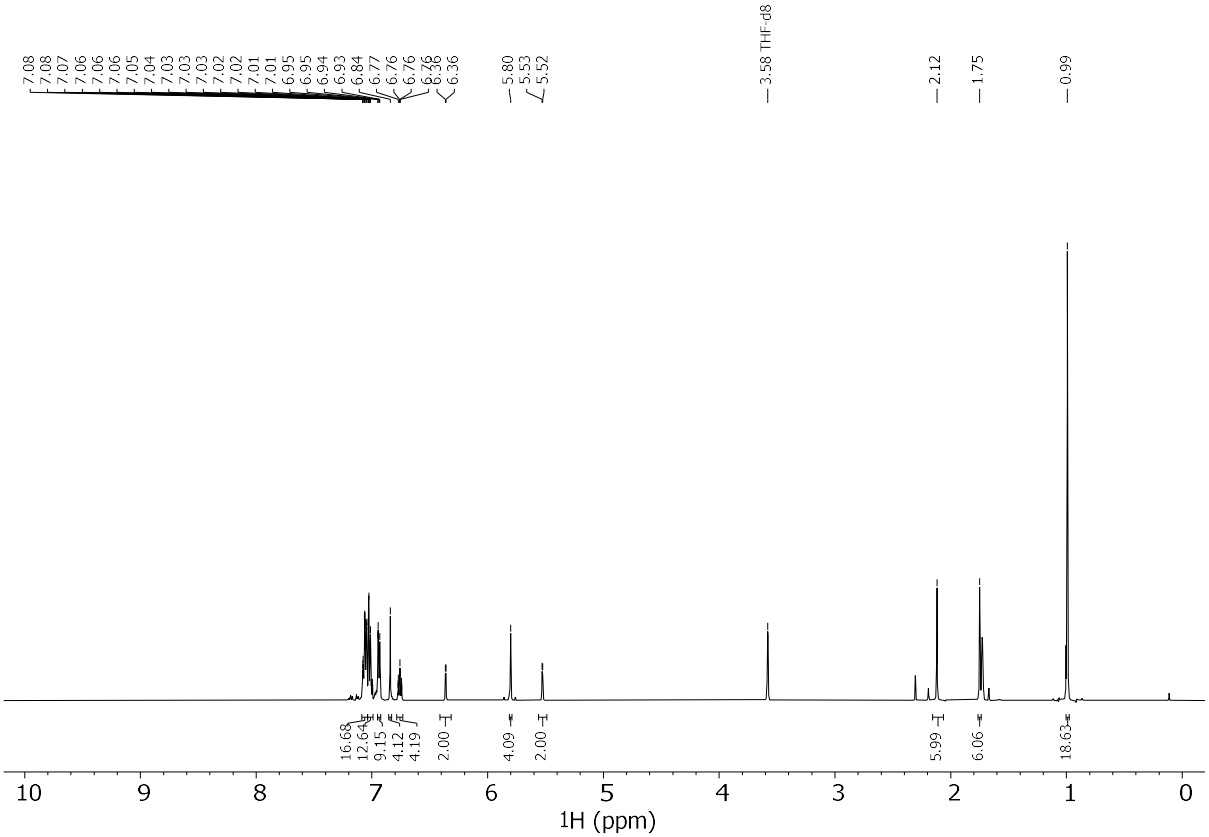


Figure S 77 *^{1}H NMR spectrum of (^{Ar*}NON)Ba in thf-d_8 at 298 K.*

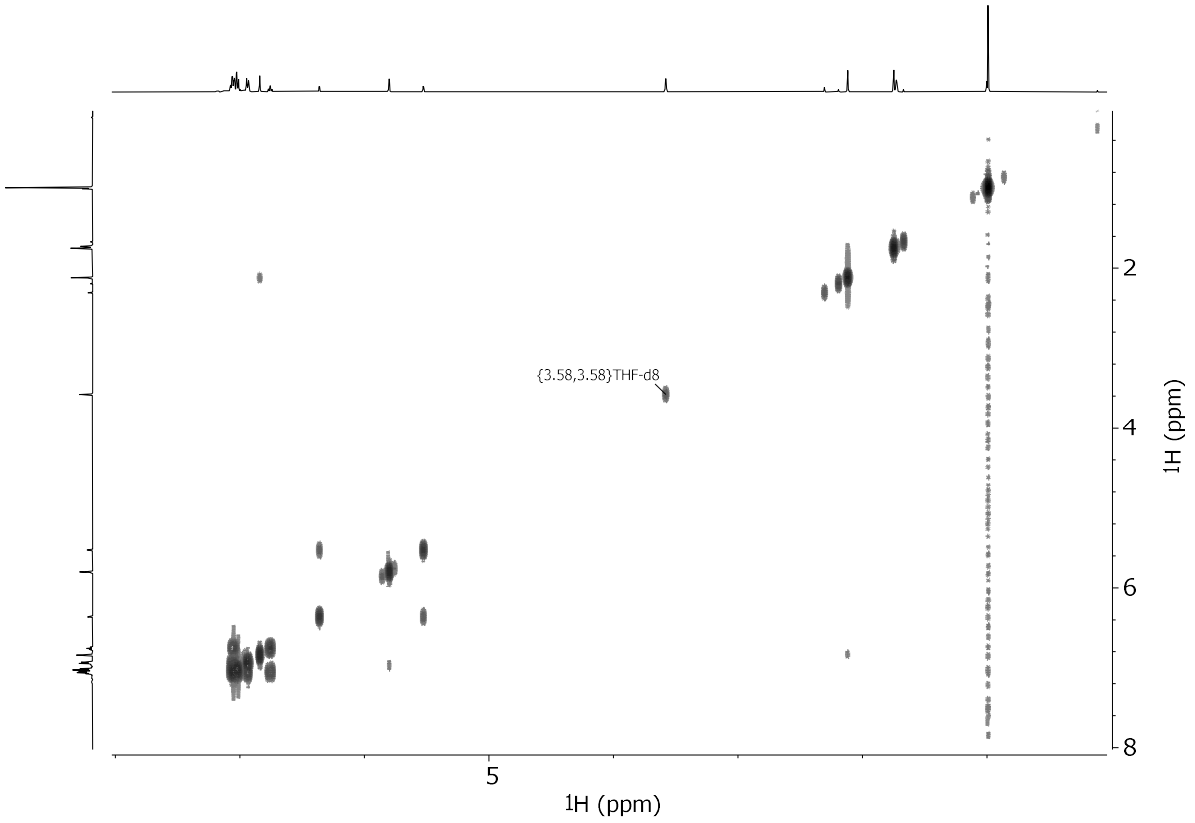


Figure S 78 *^{1}H-^{1}H COSY NMR spectrum of (^{Ar*}NON)Ba in thf-d_8 at 298 K.*

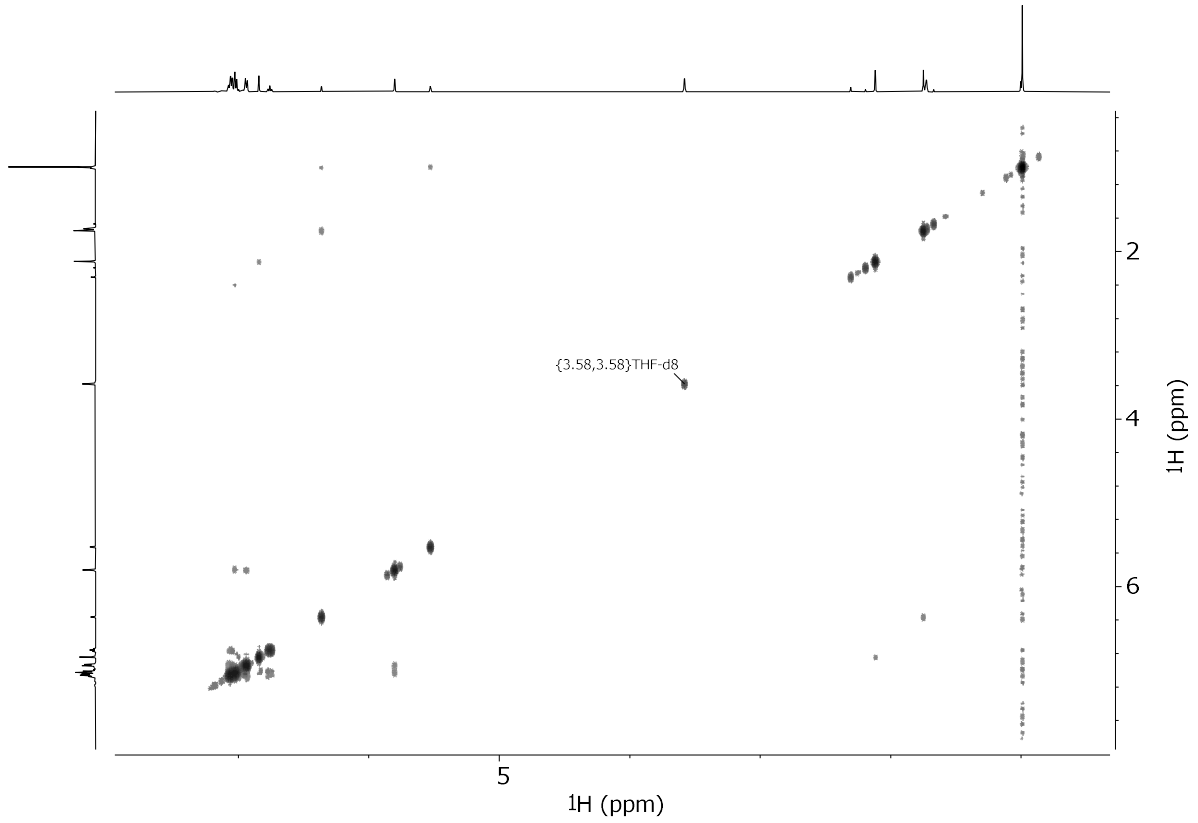


Figure S 79 *^{1}H-^{1}H NOESY NMR spectrum of (^{Ar*}NON)Ba in thf-d_8 at 298 K.*

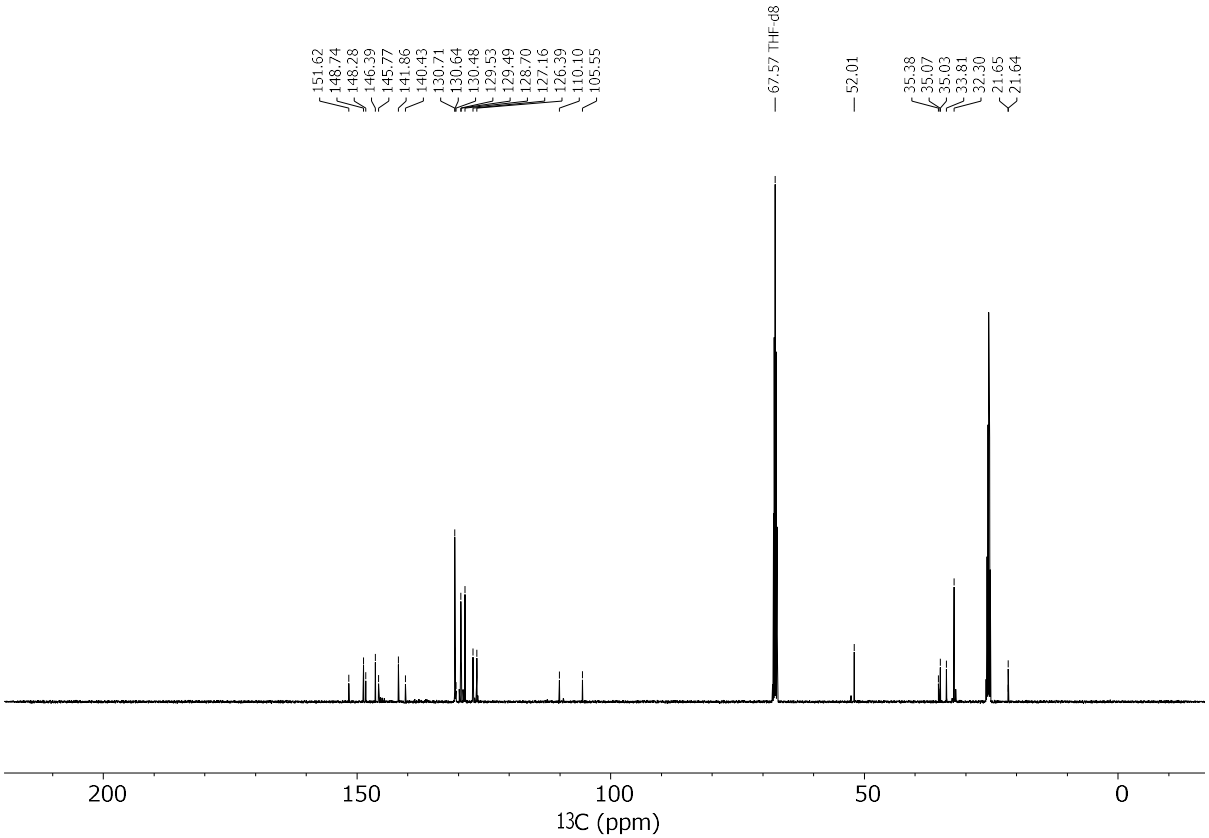


Figure S 80 *$^{13}C\{^1H\}$ NMR spectrum of (^{Ar*}NON)Ba in thf-d_8 at 298 K.*

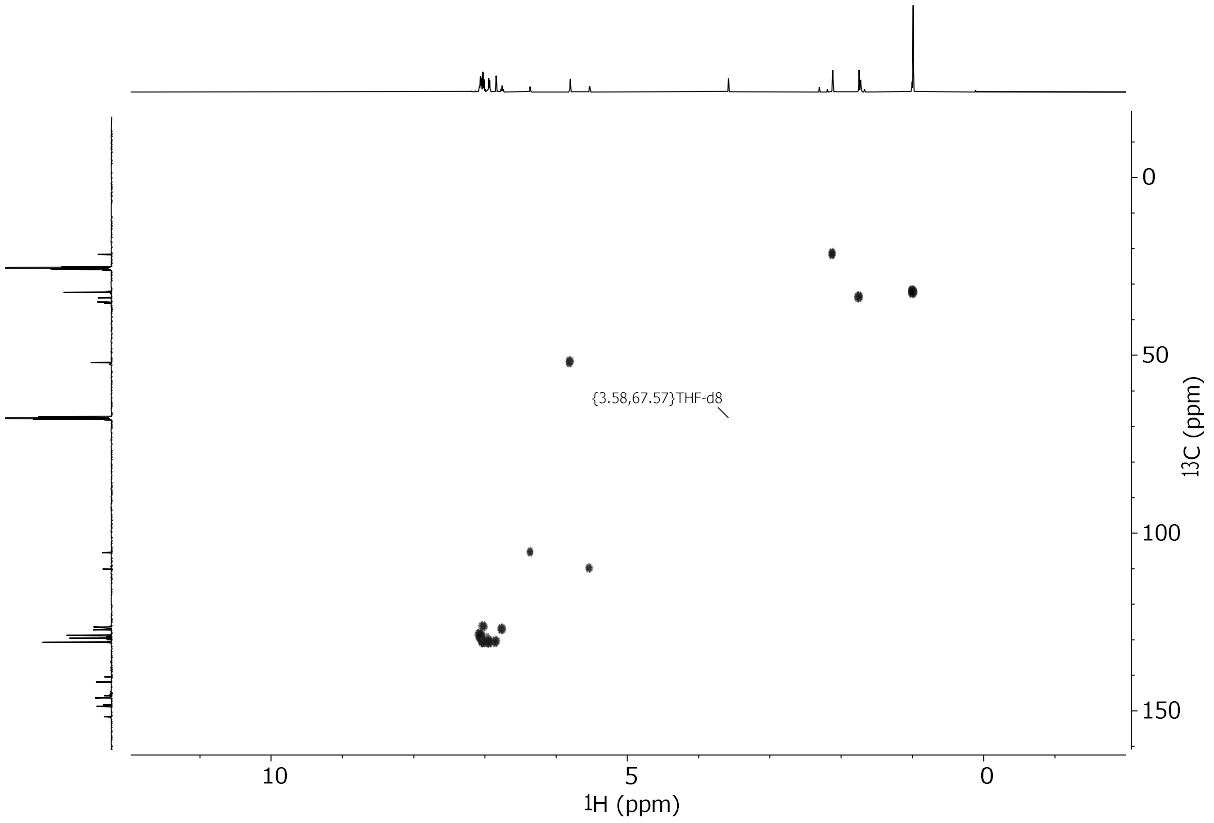


Figure S 81 *^{13}C-^{1}H HSQC NMR spectrum of (^{Ar*}NON)Ba in thf-d_8 at 298 K.*

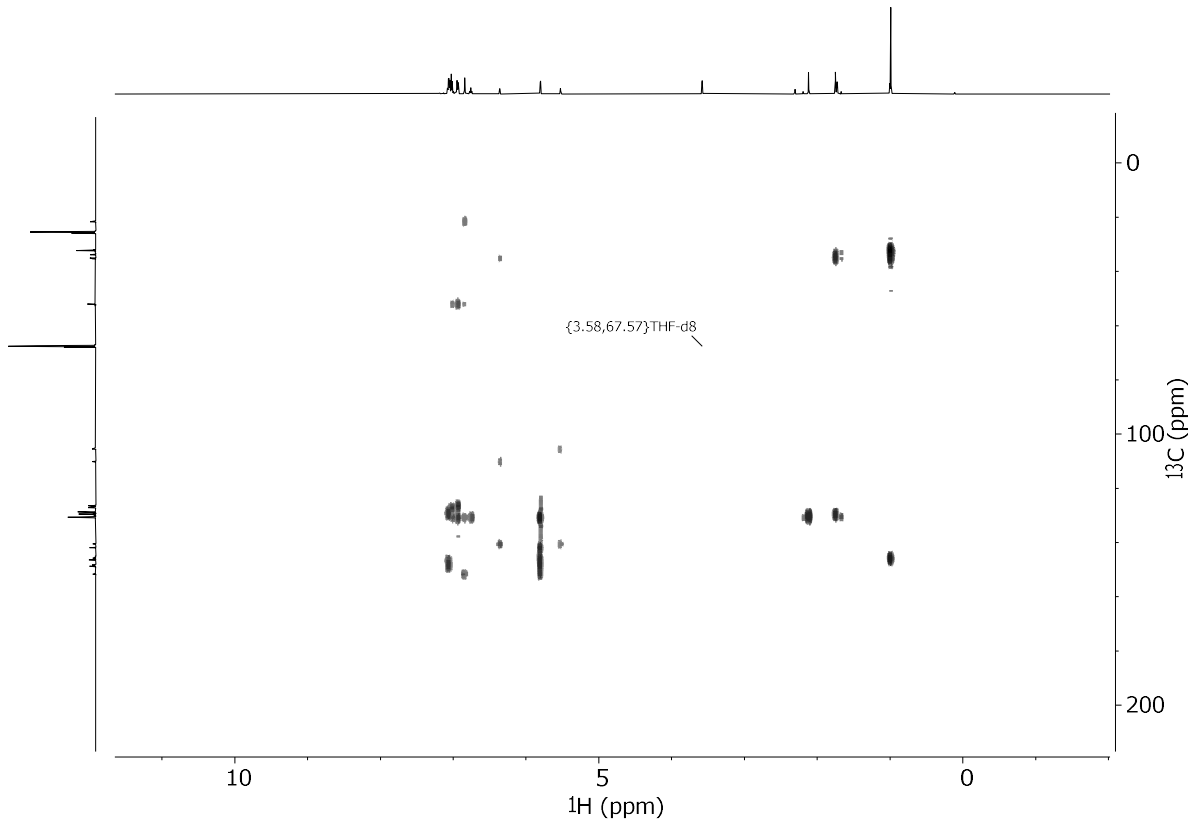


Figure S 82 *^{13}C-^{1}H HMBC NMR spectrum of (^{Ar*}NON)Ba in thf-d_8 at 298 K.*

[TMA][(^{Ar*}NON)CaF(thf)] (2-TMA)

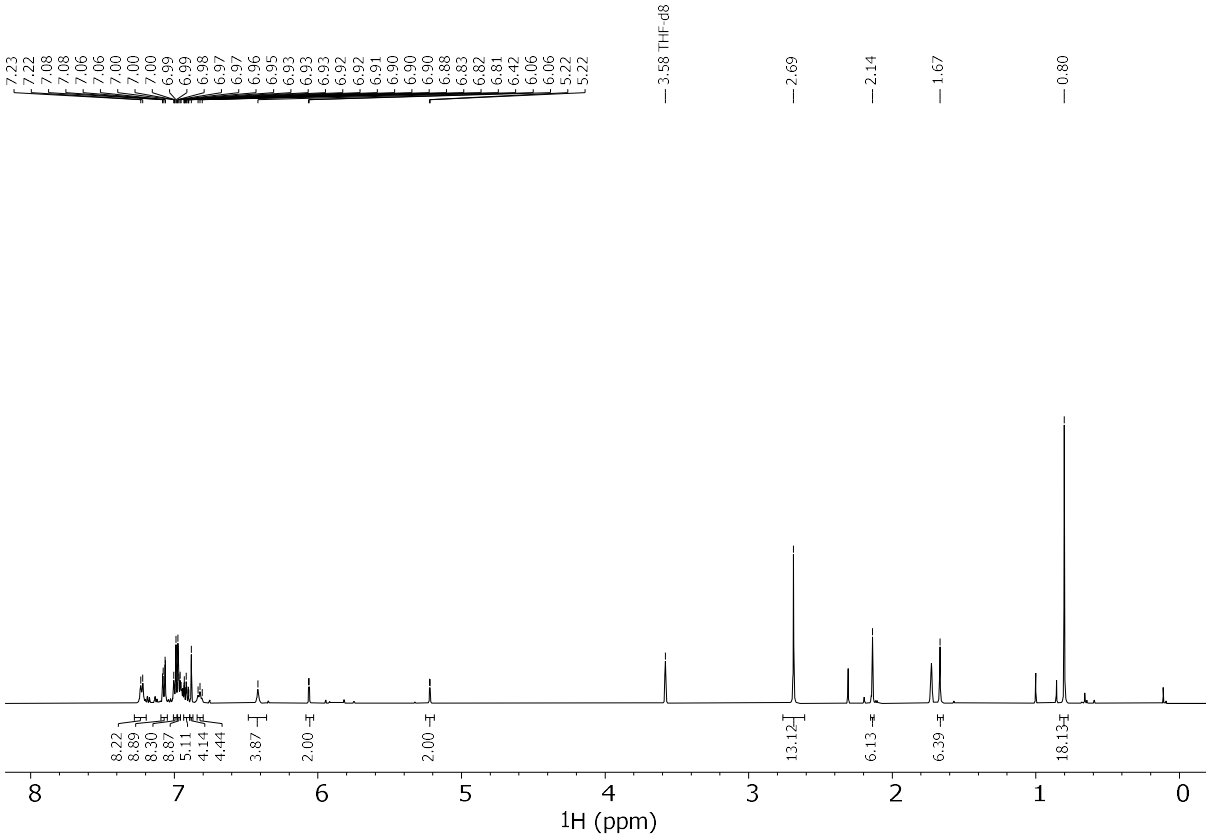


Figure S 83 *^{1}H NMR spectrum of an in-situ reaction forming **2**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the difluoride, **2**-TMA cannot be purified.*

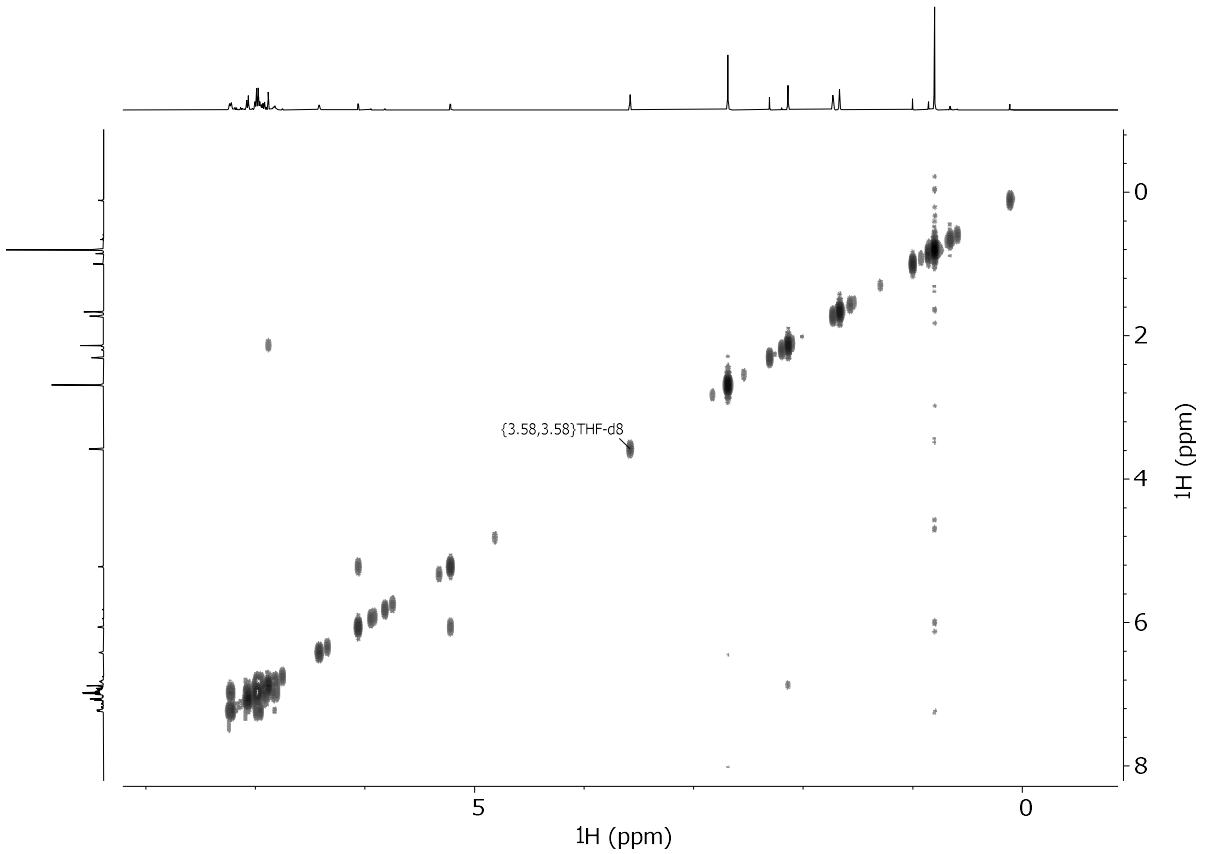


Figure S 84 *^{1}H-^{1}H COSY NMR spectrum of an in-situ reaction forming **2**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the difluoride, **2**-TMA cannot be purified.*

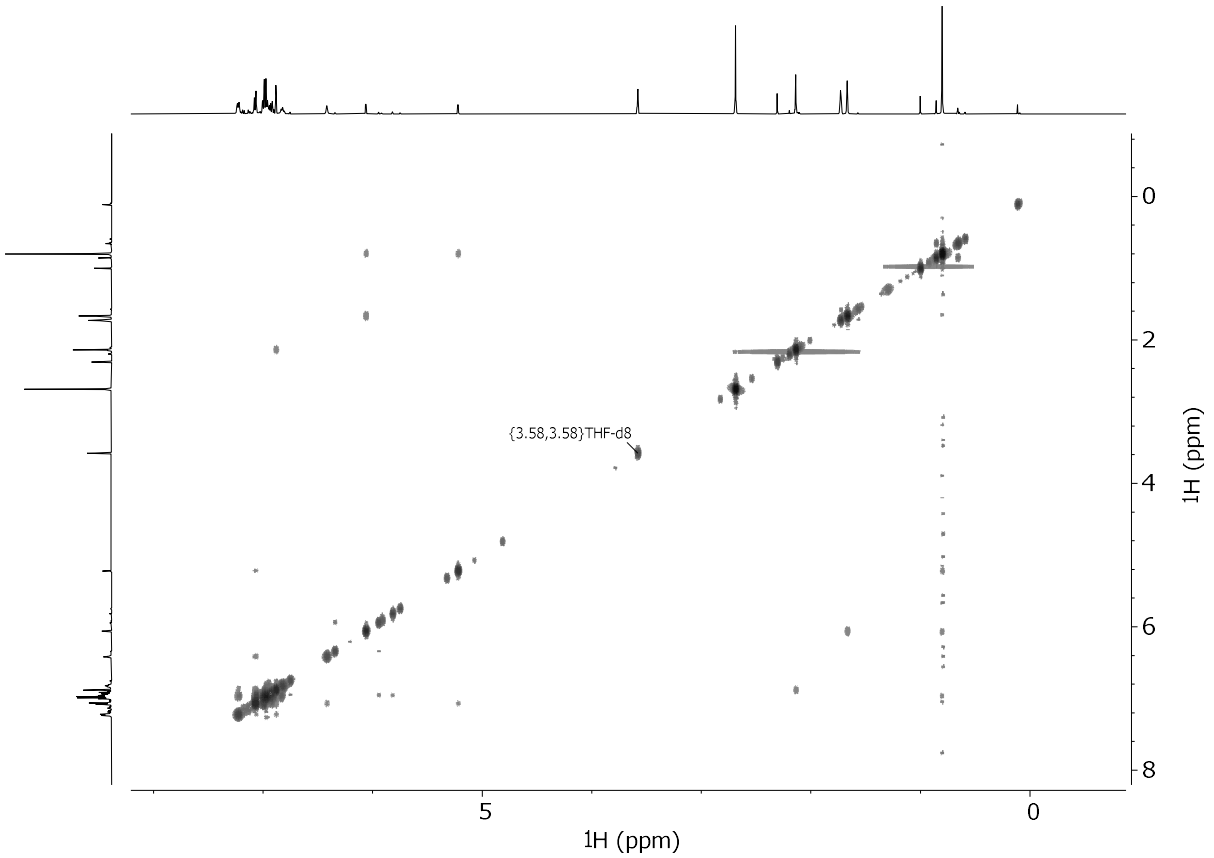


Figure S 85 *^{1}H-^{1}H ROESY NMR spectrum of an in-situ reaction forming **2**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the difluoride, **2**-TMA cannot be purified.*

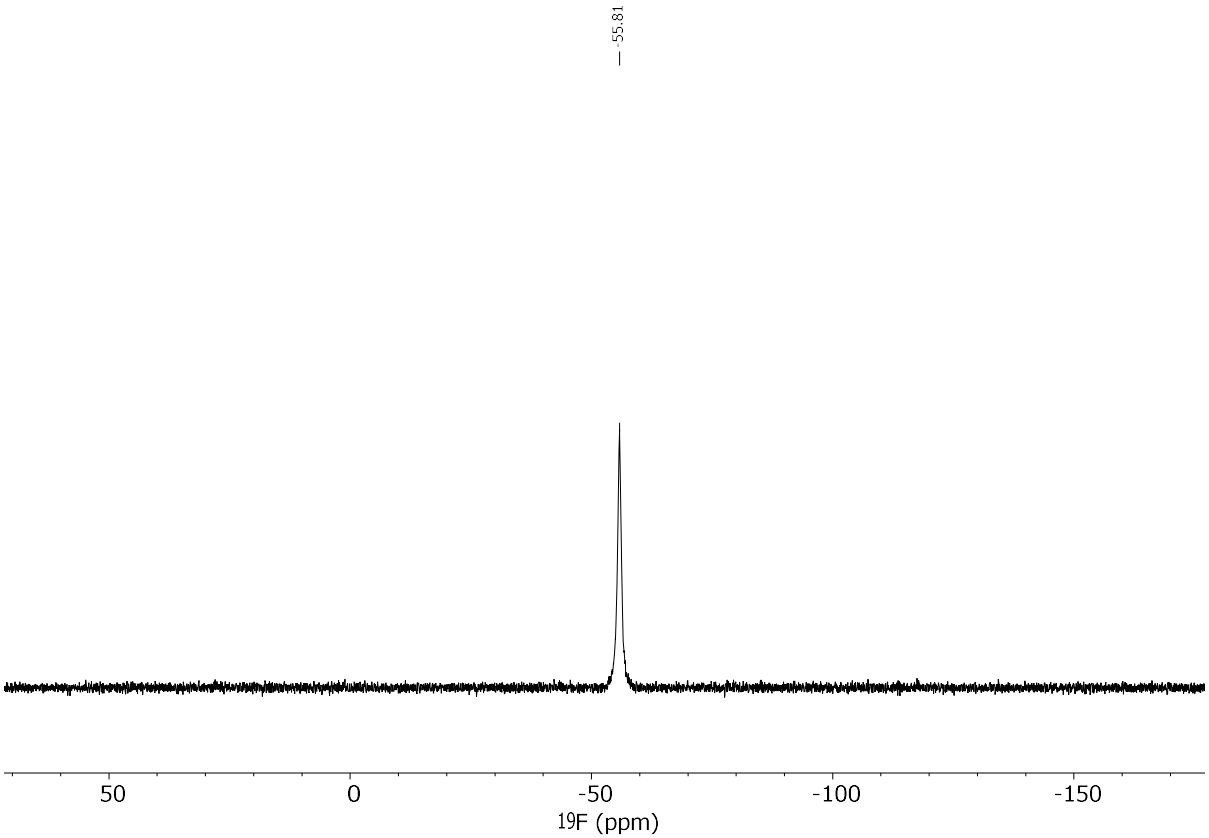


Figure S 86 *^{19}F NMR spectrum of an in-situ reaction forming **2**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the difluoride, **2**-TMA cannot be purified.*

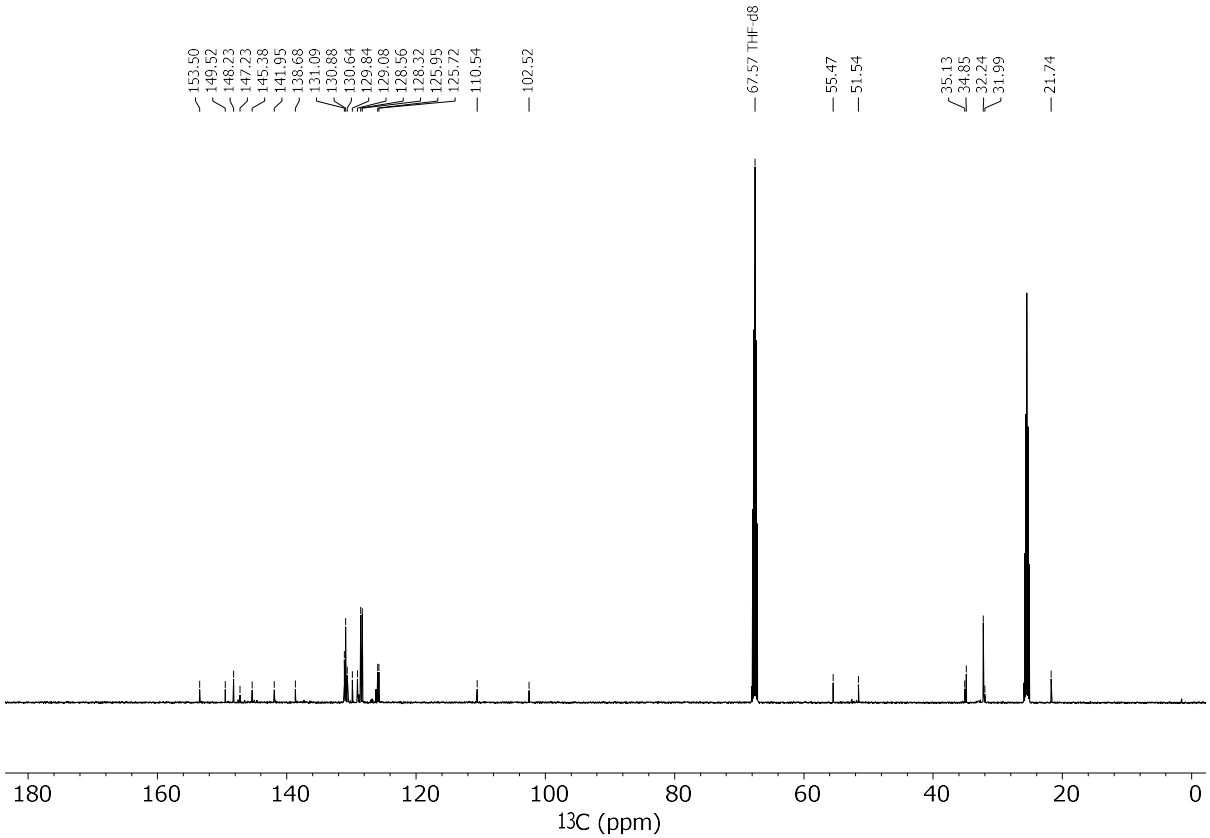


Figure S 87 *$^{13}C\{^{1}H\}$ NMR spectrum of an in-situ reaction forming **2**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the difluoride, **2**-TMA cannot be purified.*

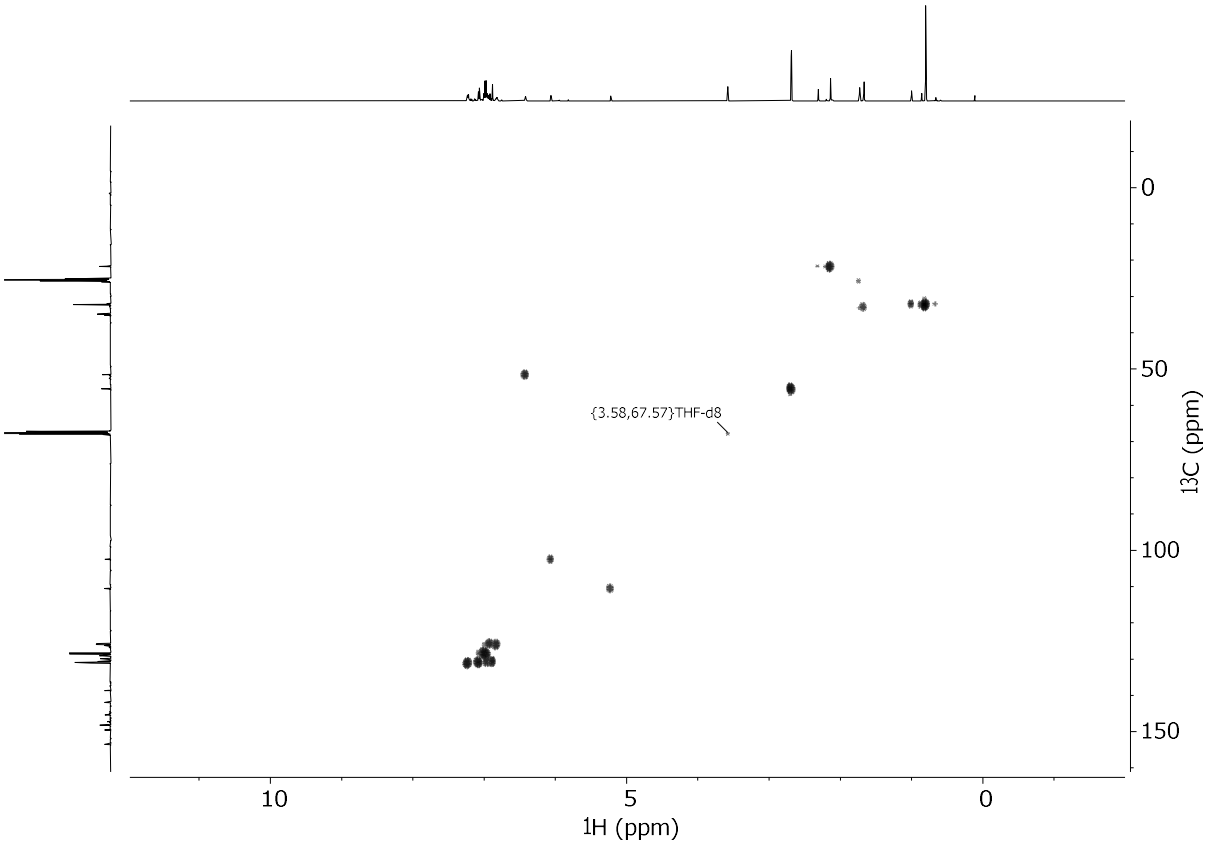


Figure S 88 *^{13}C-^{1}H HSQC NMR spectrum of an in-situ reaction forming **2**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the difluoride, **2**-TMA cannot be purified.*

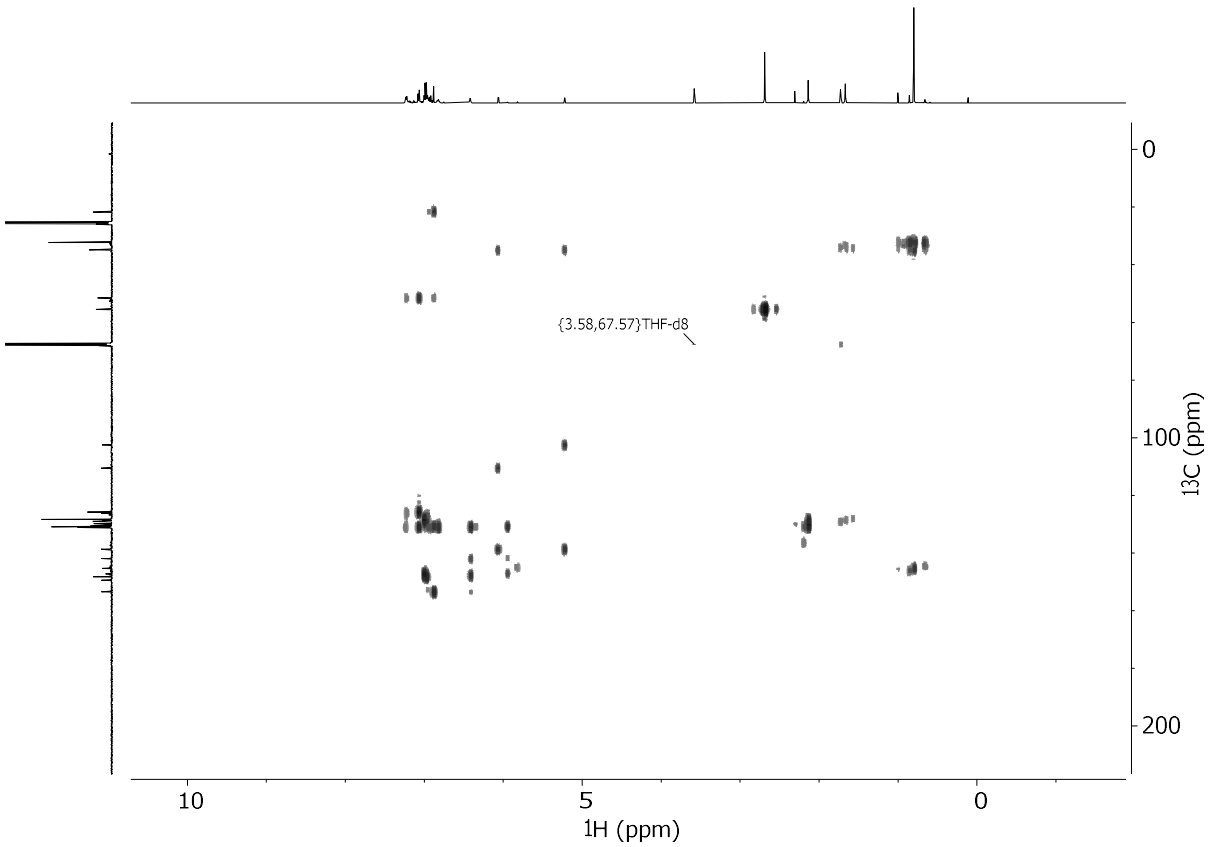


Figure S 89 *^{13}C-^{1}H HMBC NMR spectrum of an in-situ reaction forming **2**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the difluoride, **2**-TMA cannot be purified.*

[PPh$_4$][(^{Ar*}NON)CaF(thf)] (2-PPh$_4$)

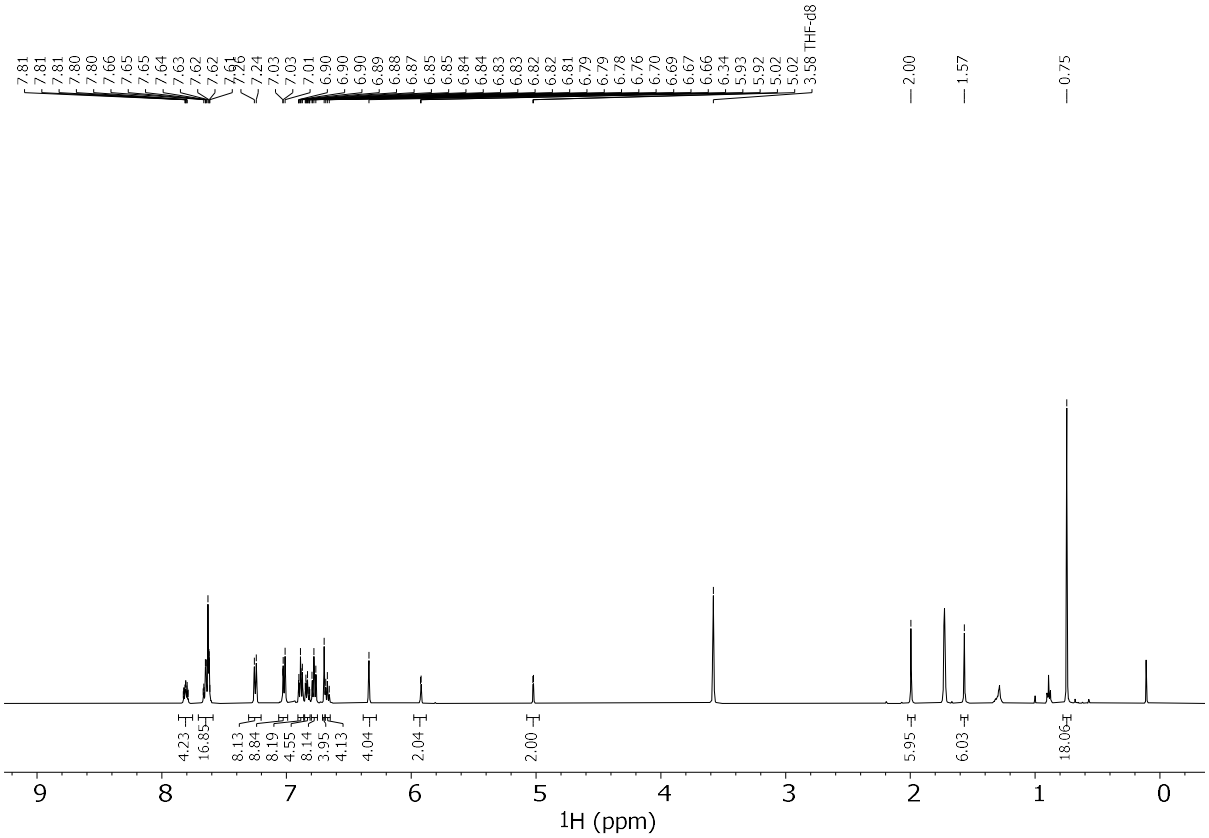


Figure S 90 *^{1}H NMR spectrum of **2**-PPh$_4$ in thf-d$_8$ at 298 K.*

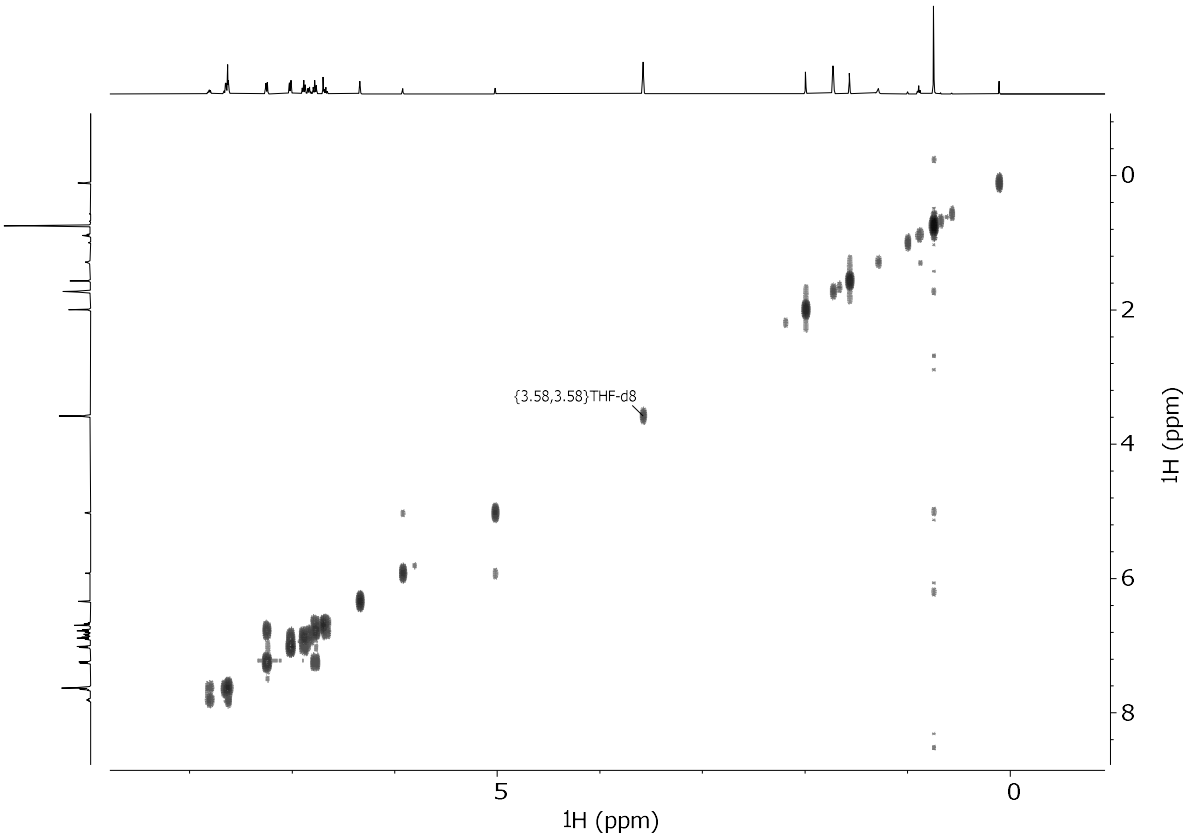


Figure S 91 *^{1}H-^{1}H COSY NMR spectrum of **2**-PPh_4 in thf-d_8 at 298 K.*

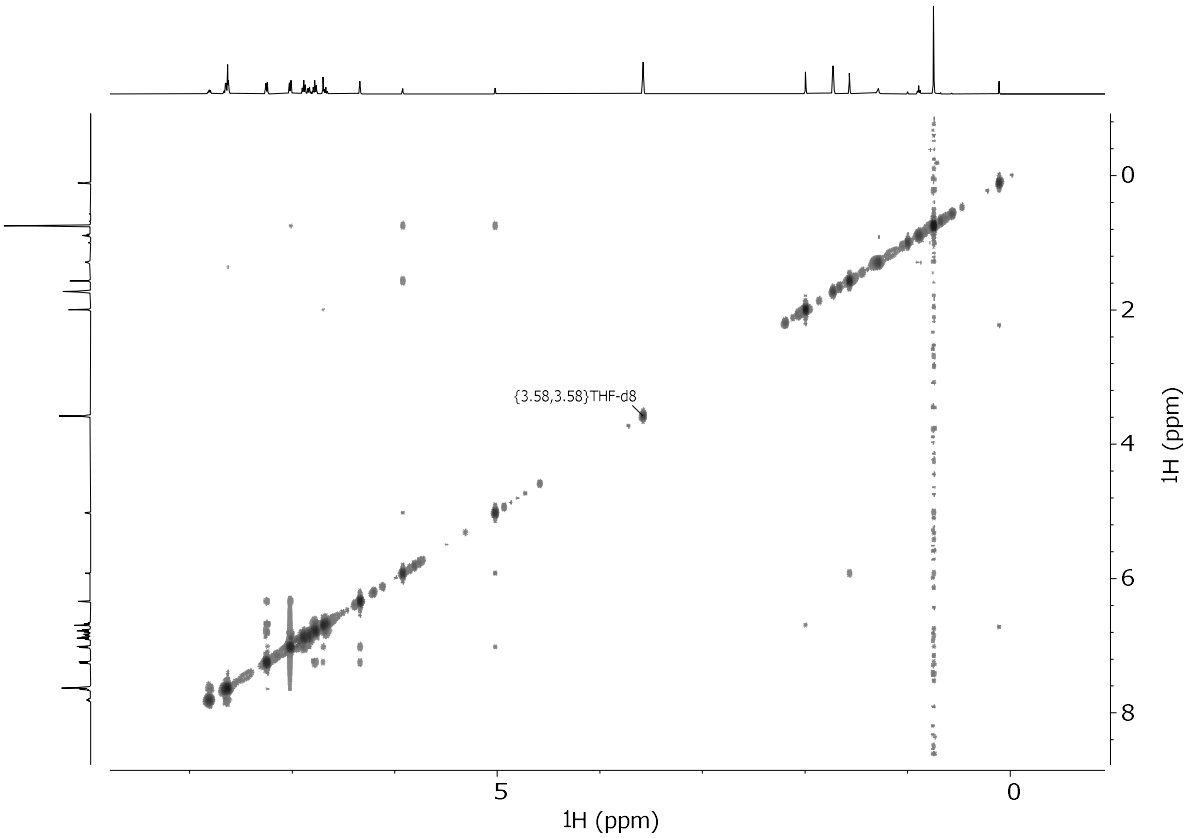


Figure S 92 *^{1}H-^{1}H NOESY NMR spectrum of **2**-PPh_4 in thf-d_8 at 298 K.*

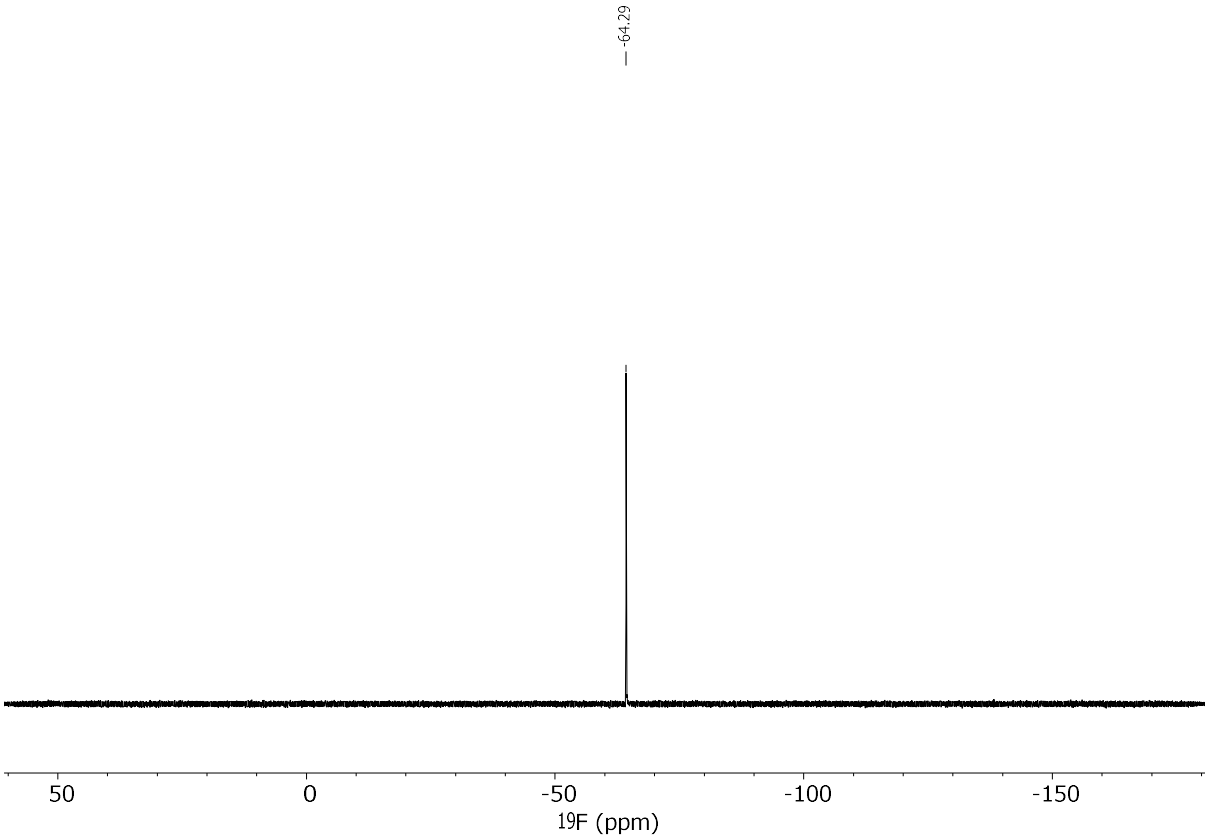


Figure S 93 *^{19}F NMR spectrum of **2**-PPh_4 in thf-d_8 at 298 K.*

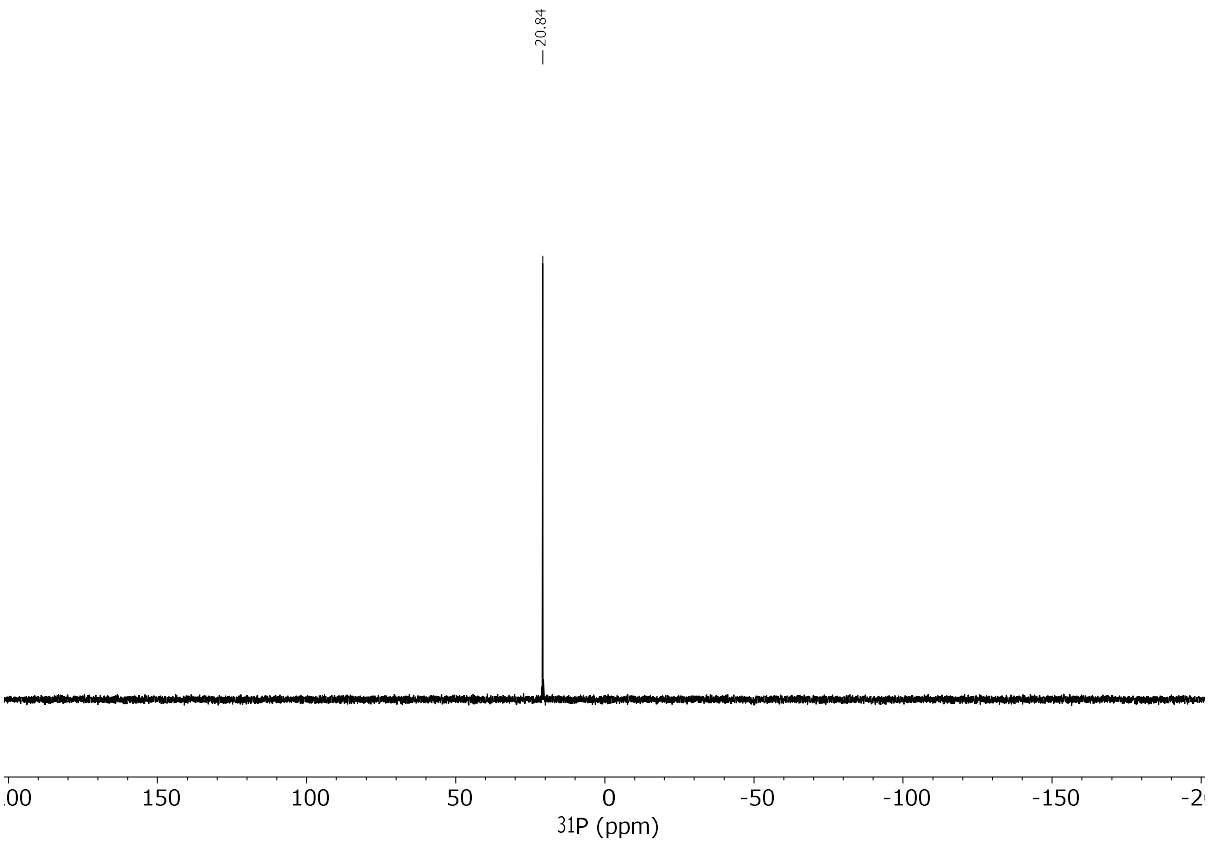


Figure S 94 *^{31}P NMR spectrum of **2**-PPh_4 in thf-d_8 at 298 K.*

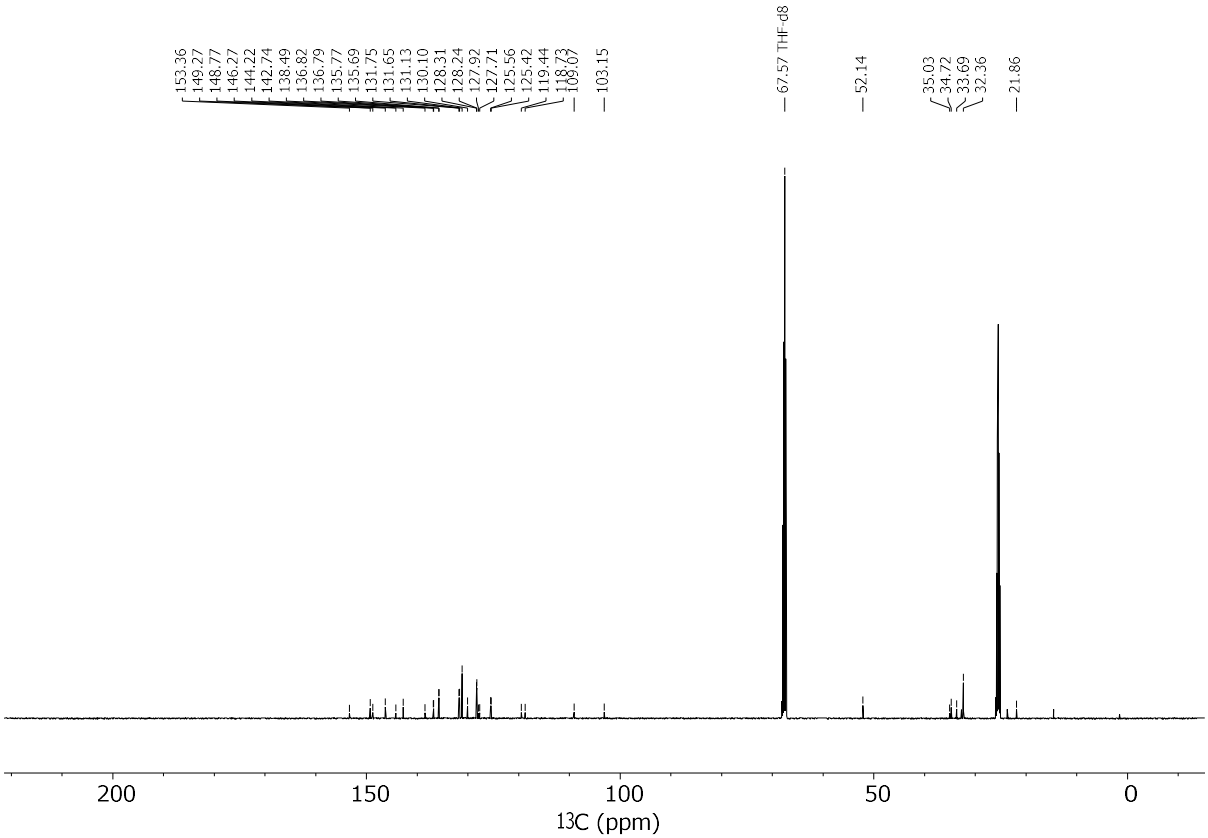


Figure S 95 *$^{13}C\{^{1}H\}$ NMR spectrum of **2**-PPh_4 in thf-d_8 at 298 K.*

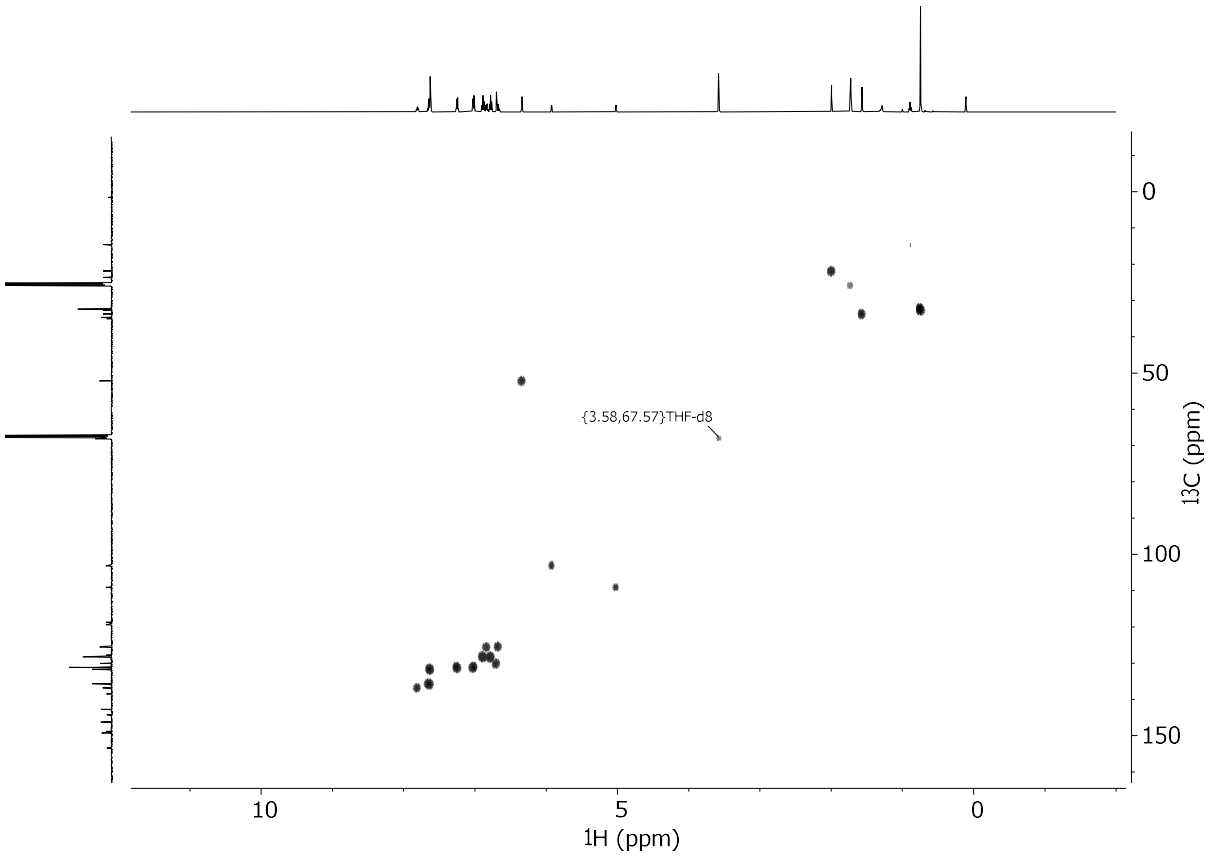


Figure S 96 *^{13}C-^{1}H HSQC NMR spectrum of **2**-PPh_4 in thf-d_8 at 298 K.*

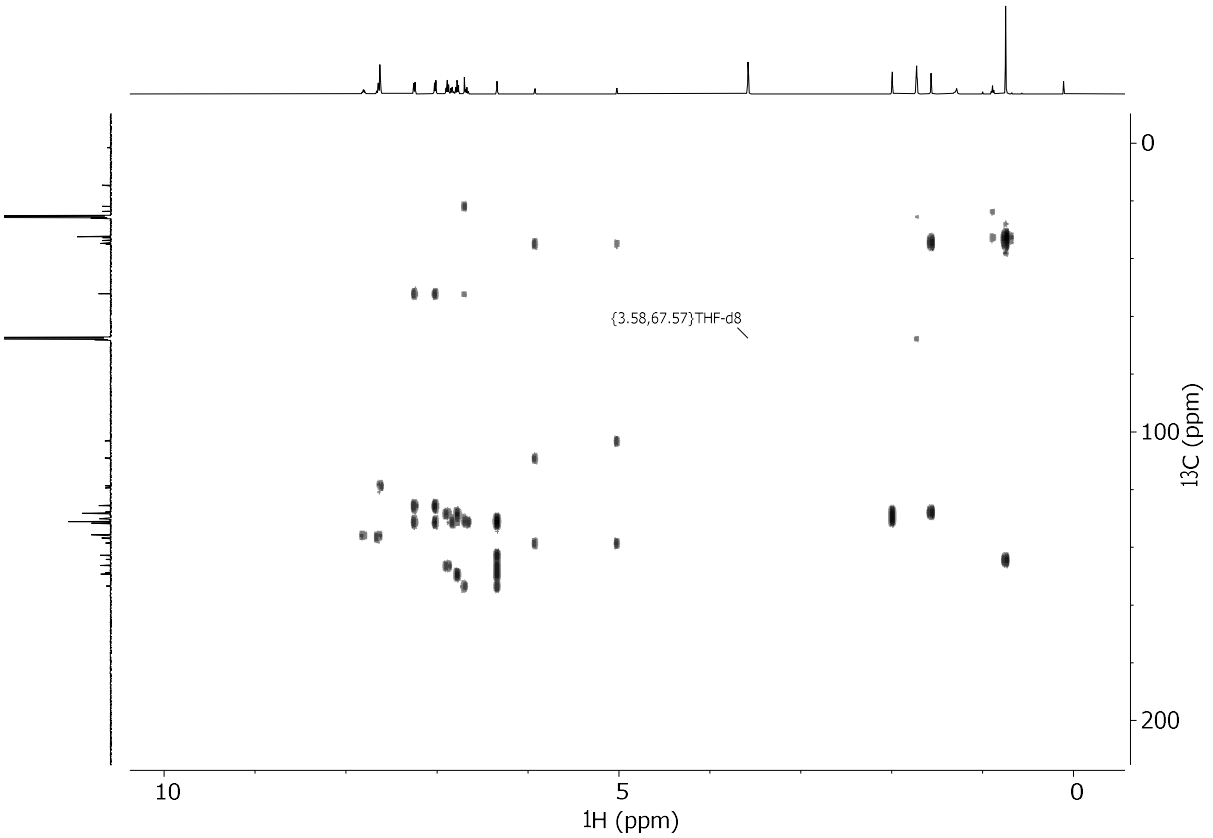


Figure S 97 *^{13}C-^{1}H HMBC NMR spectrum of **2**-PPh_4 in thf-d_8 at 298 K.*

[TMA]$_2$[(^{Ar*}NON)CaF$_2$] (3-TMA$_2$)

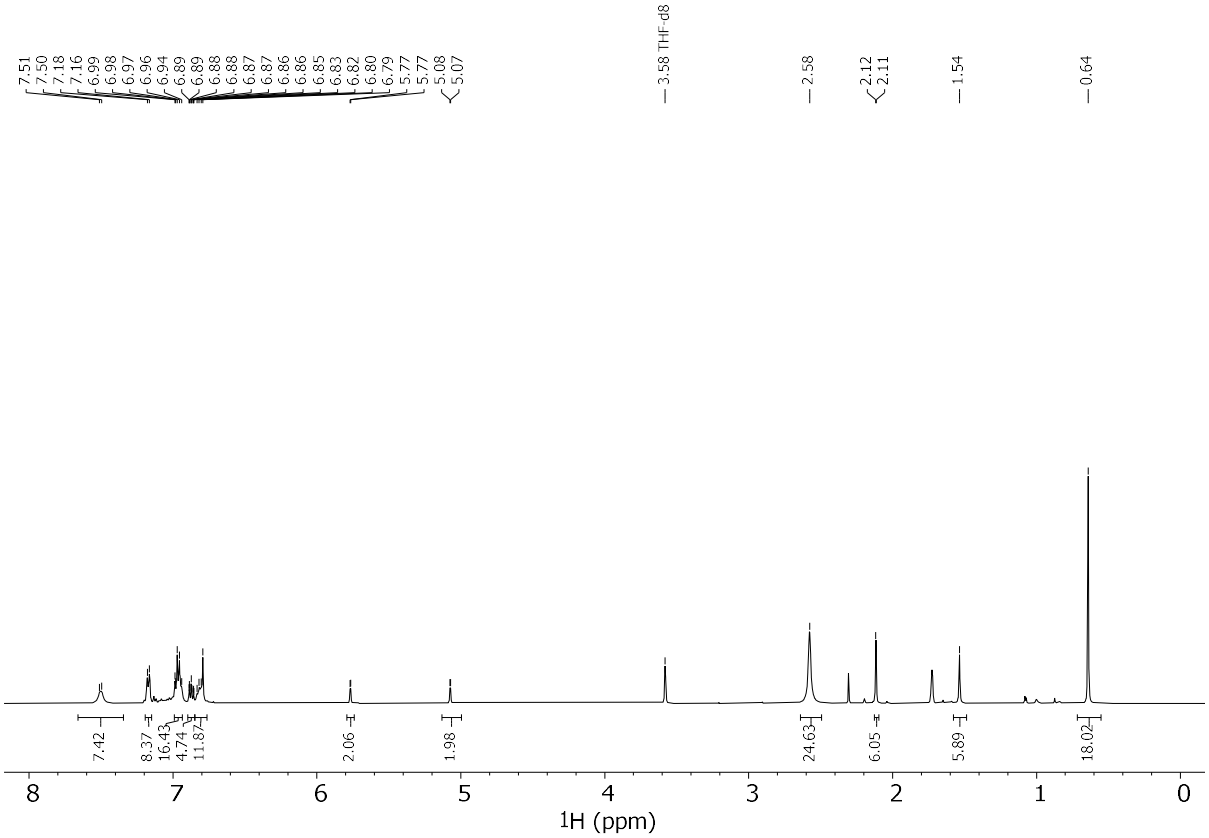


Figure S 98 *^{1}H NMR spectrum of **3**-TMA$_2$ in thf-d$_8$ at 298 K.*

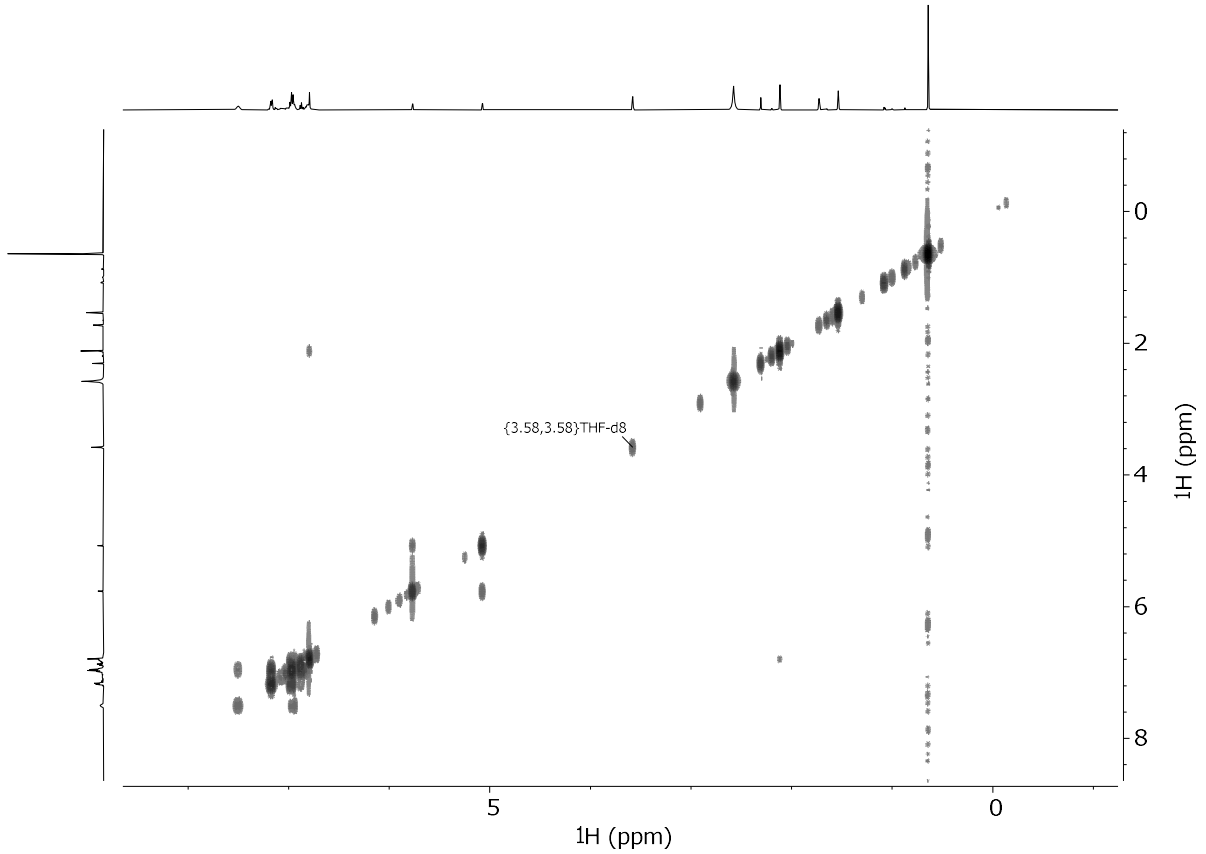


Figure S 99 *^{1}H-^{1}H COSY NMR spectrum of **3**-TMA$_2$ in thf-d$_8$ at 298 K.*

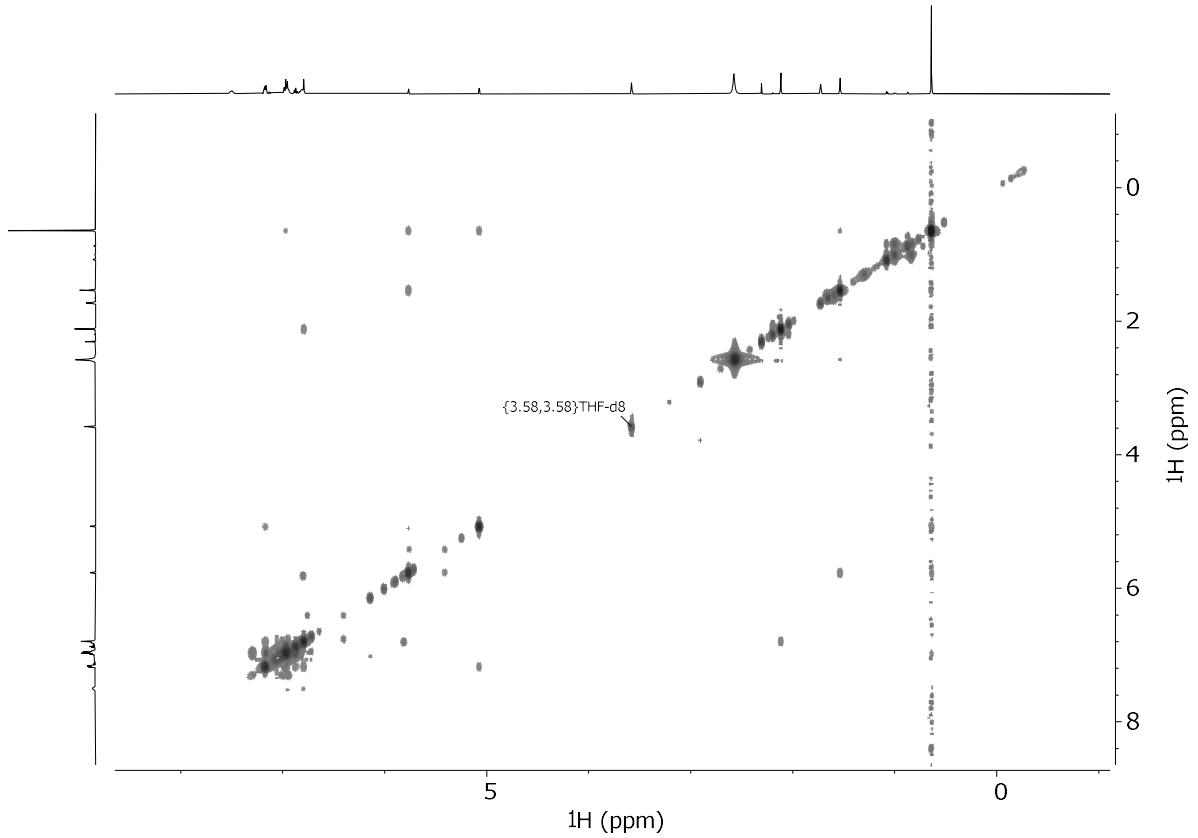


Figure S 100 *^{1}H-^{1}H NOESY NMR spectrum of **3**-TMA$_2$ in thf-d$_8$ at 298 K.*

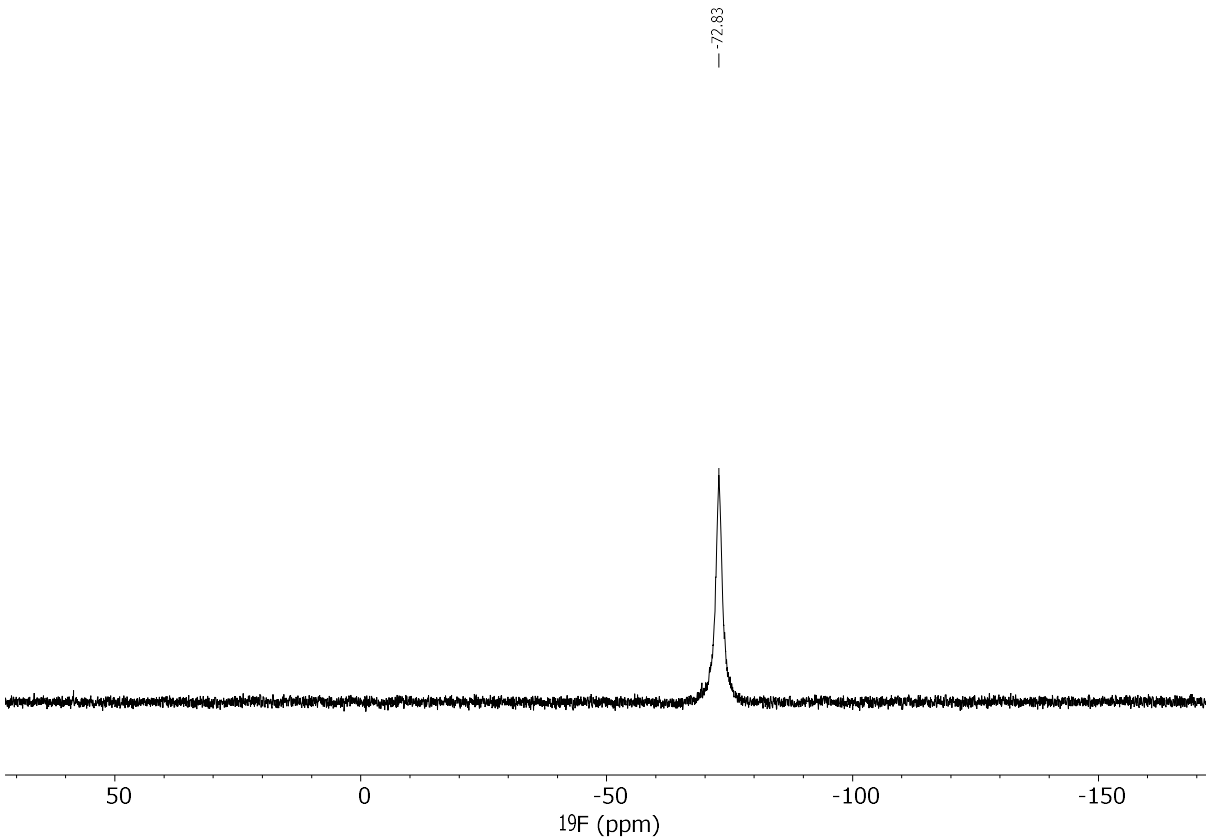


Figure S 101 *^{19}F NMR spectrum of **3**-TMA$_2$ in thf-d$_8$ at 298 K.*

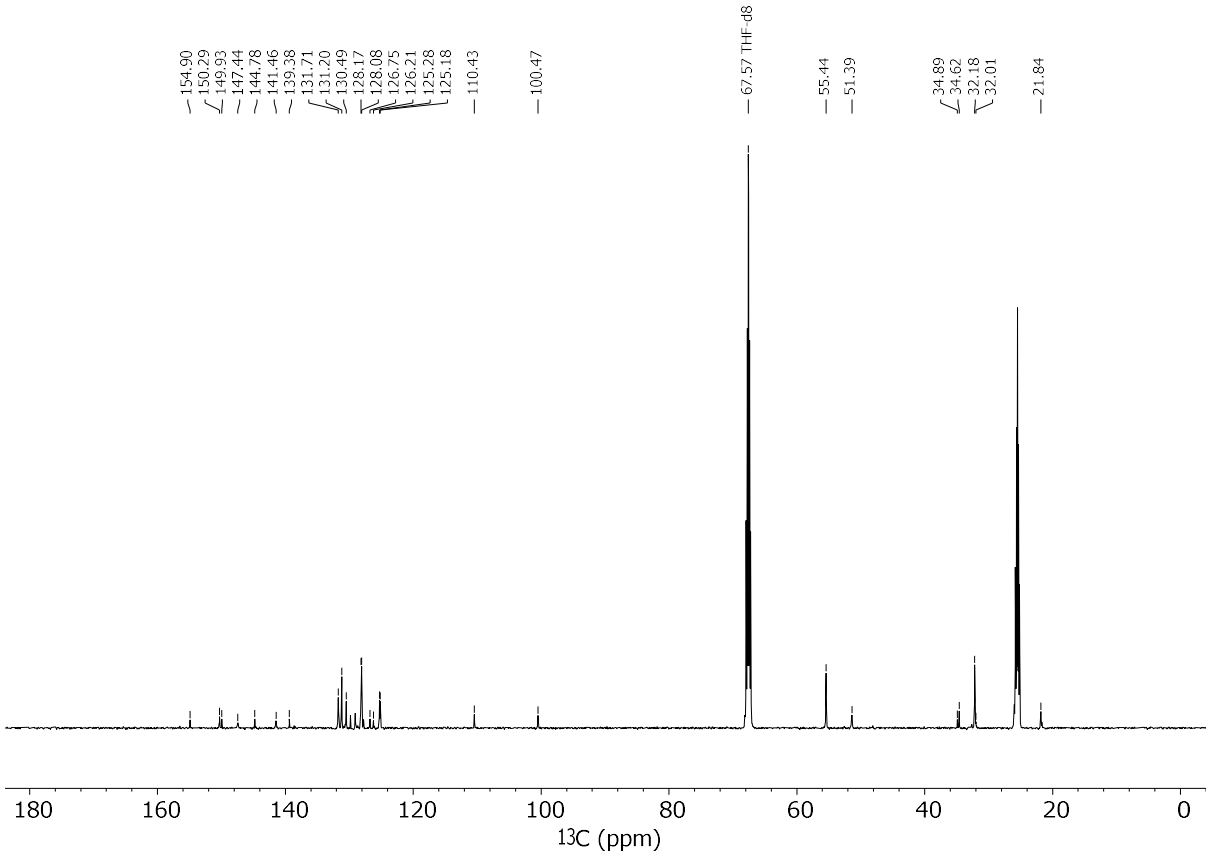


Figure S 102 *$^{13}C\{^{1}H\}$ NMR spectrum of **3**-TMA_2 in thf-d_8 at 298 K.*

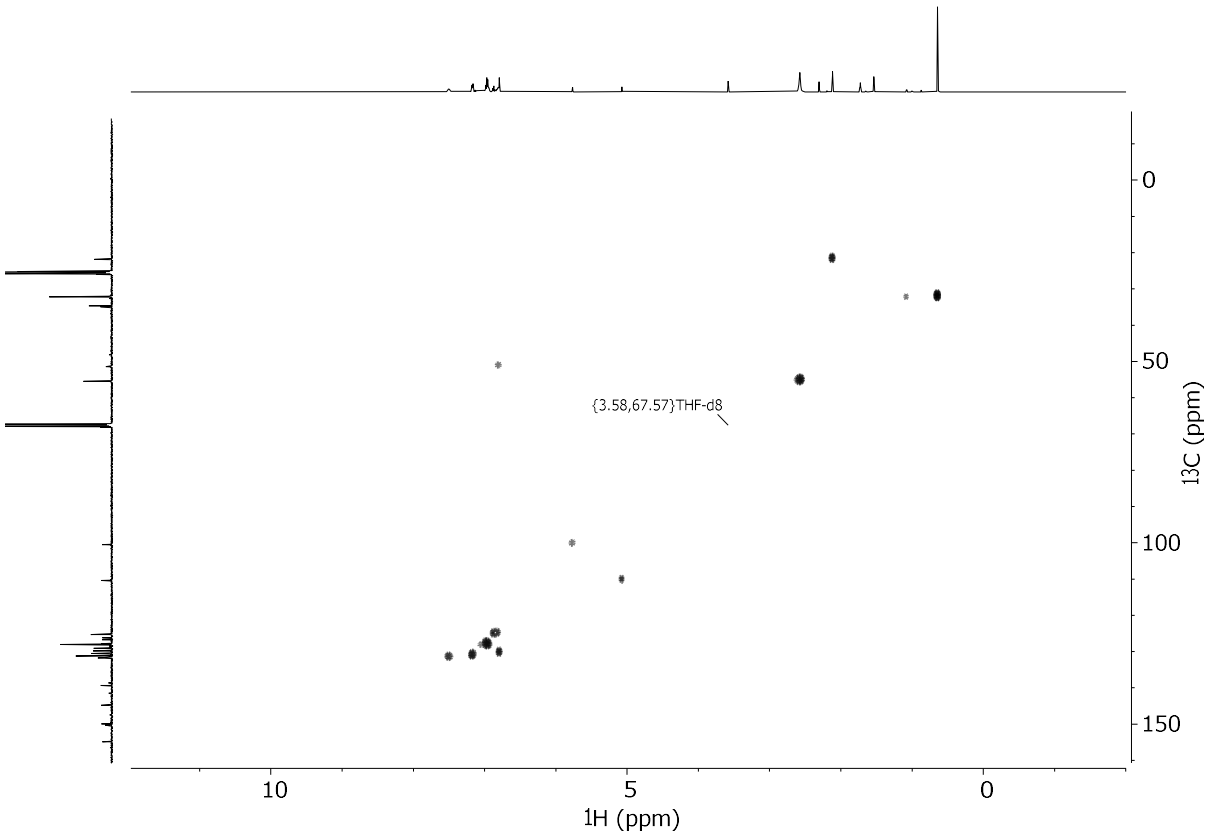


Figure S 103 *^{13}C-^{1}H HSQC NMR spectrum of **3**-TMA_2 in thf-d_8 at 298 K.*

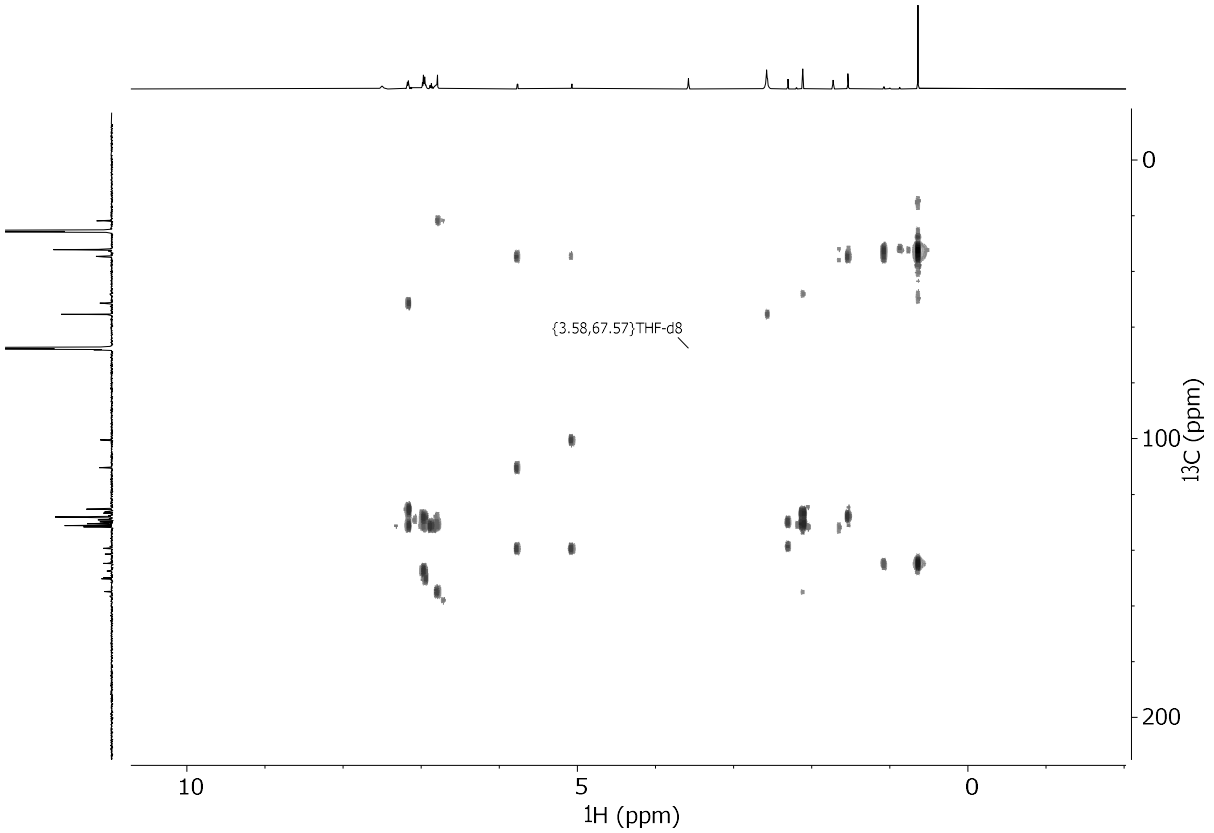


Figure S 104 *^{13}C-^{1}H HMBC NMR spectrum of **3**-TMA_2 in thf-d_8 at 298 K.*

$[PPh_4]_2[(Ar^*NON)CaF_2]$ (3-$(PPh_4)_2$)

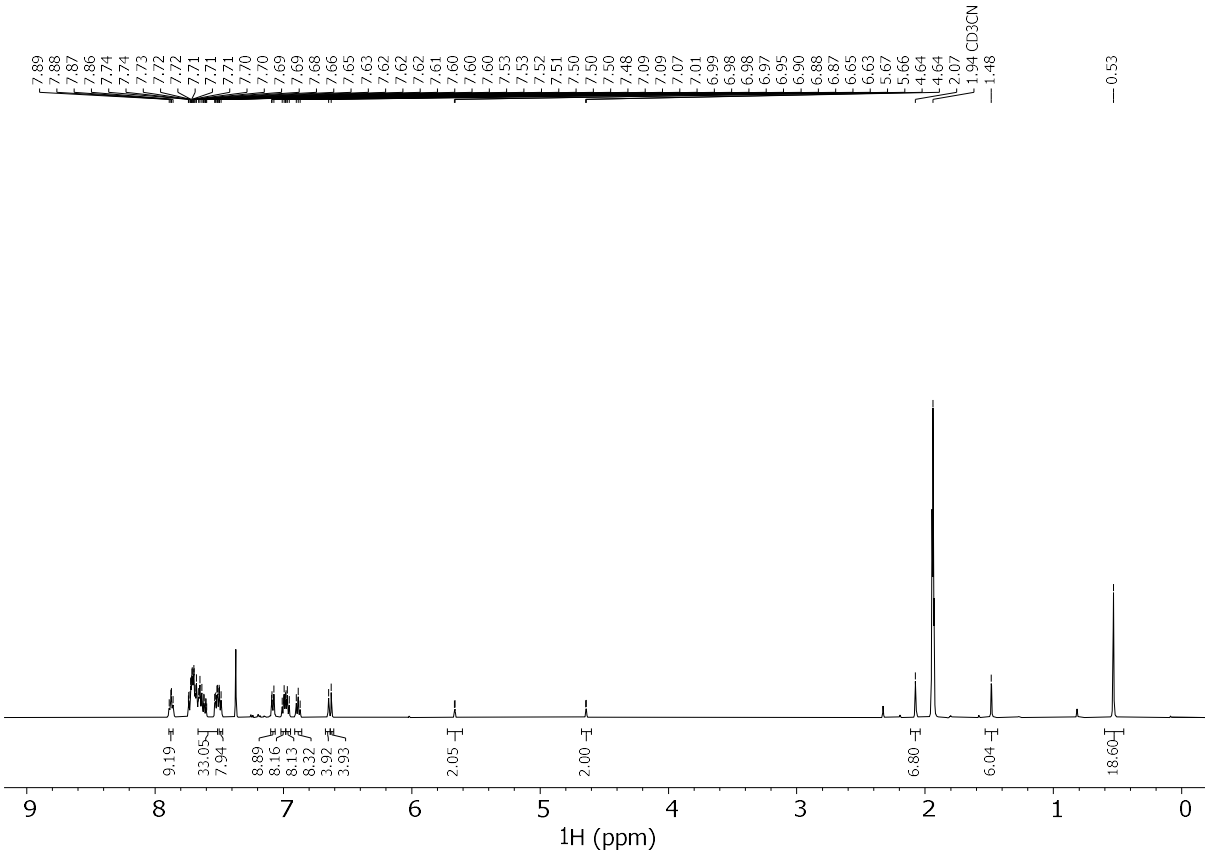


Figure S 105 *^{1}H NMR spectrum of **3**-$(PPh_4)_2$ in MeCN-d_3 at 298 K.*

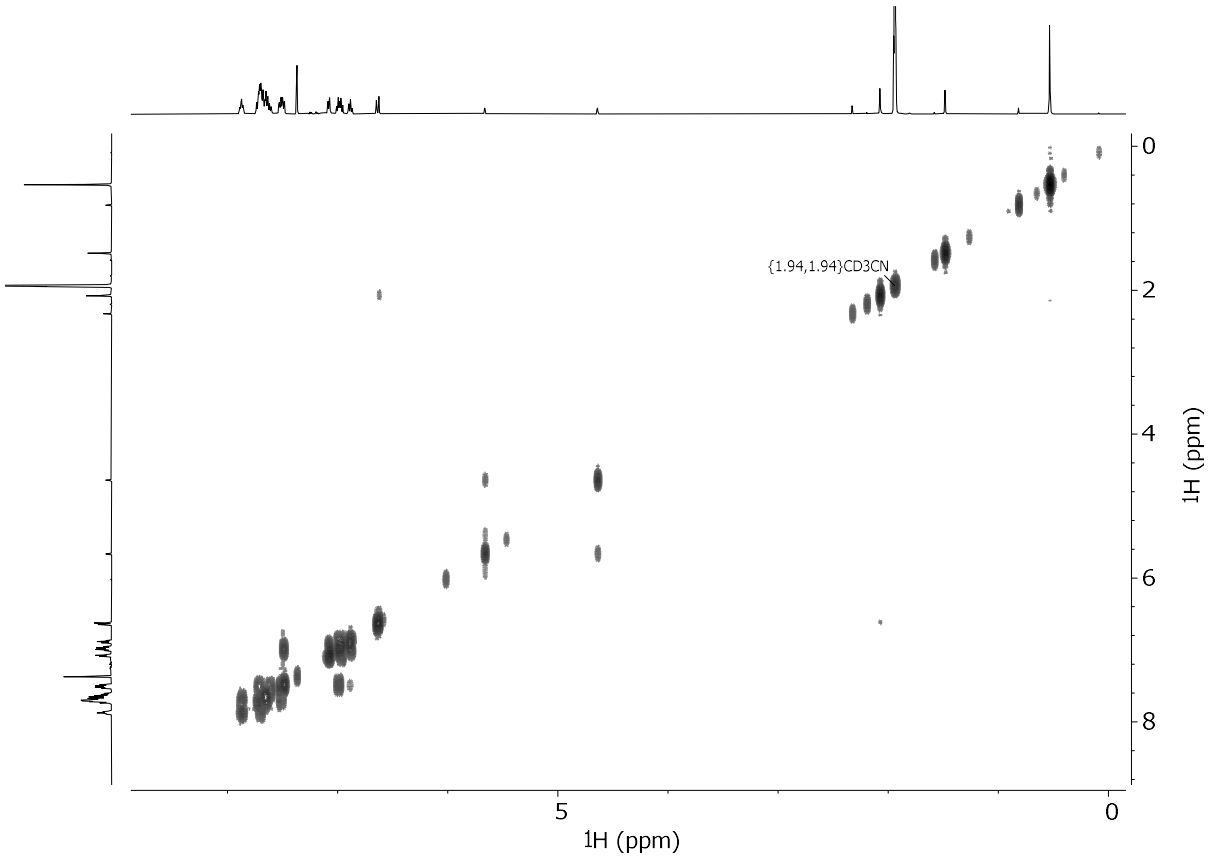


Figure S 106 *^{1}H-^{1}H COSY NMR spectrum of **3**-$(PPh_4)_2$ in MeCN-d_3 at 298 K.*

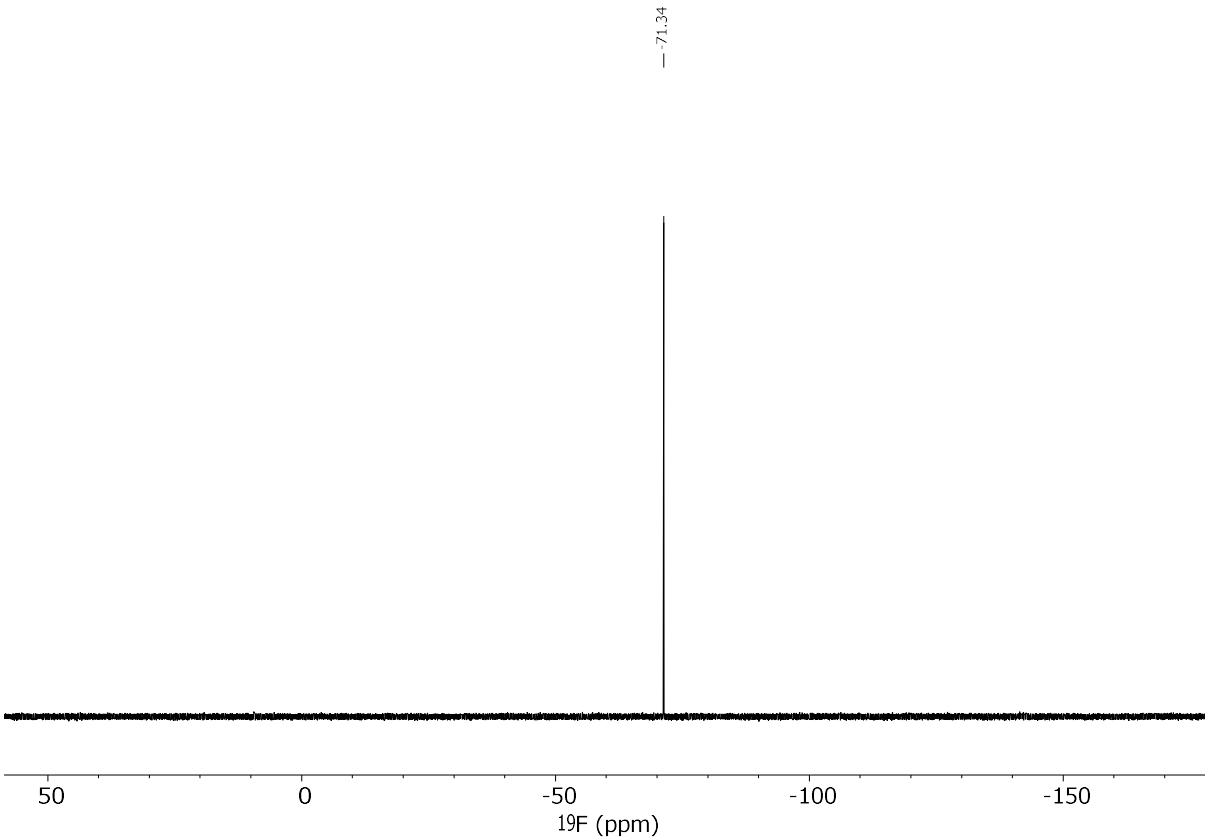


Figure S 107 *^{19}F NMR spectrum of **3**-$(PPh_4)_2$ in MeCN-d_3 at 298 K.*

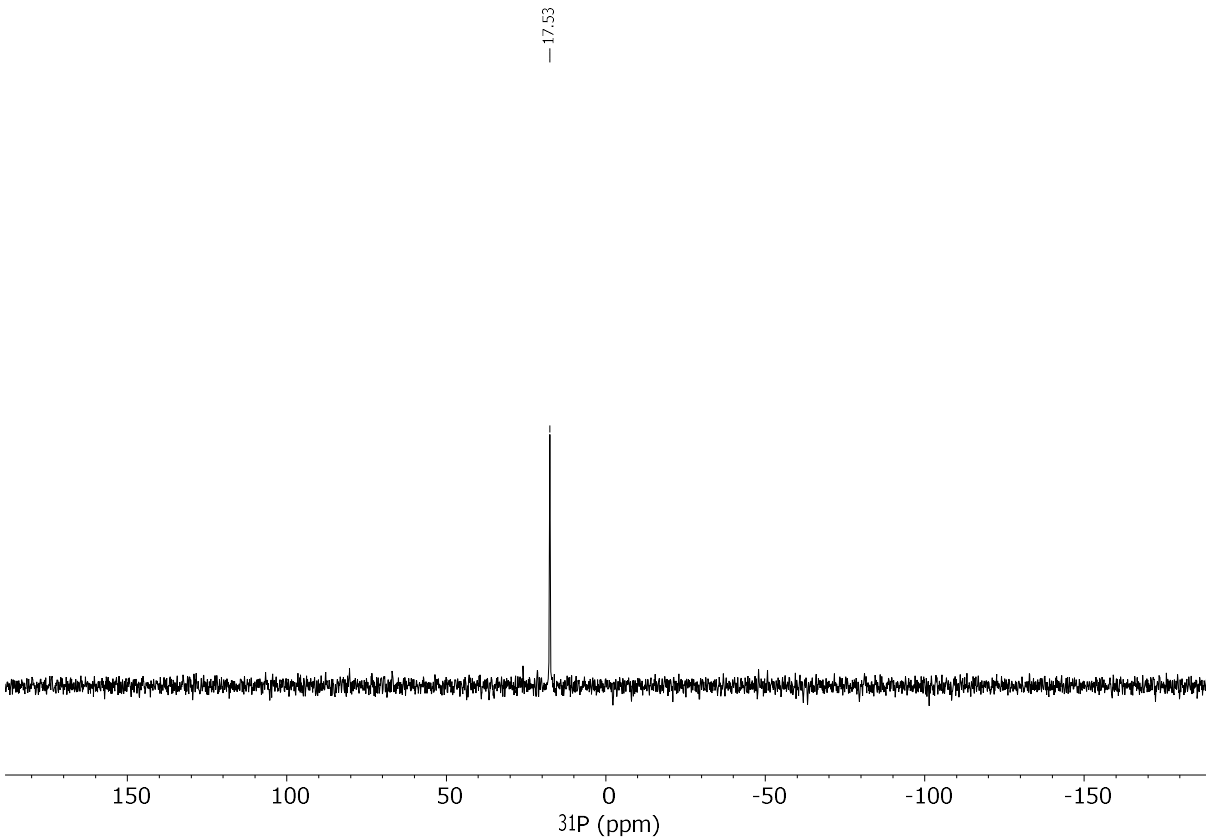


Figure S 108 *^{31}P NMR spectrum of **3**-$(PPh_4)_2$ in MeCN-d_3 at 298 K.*

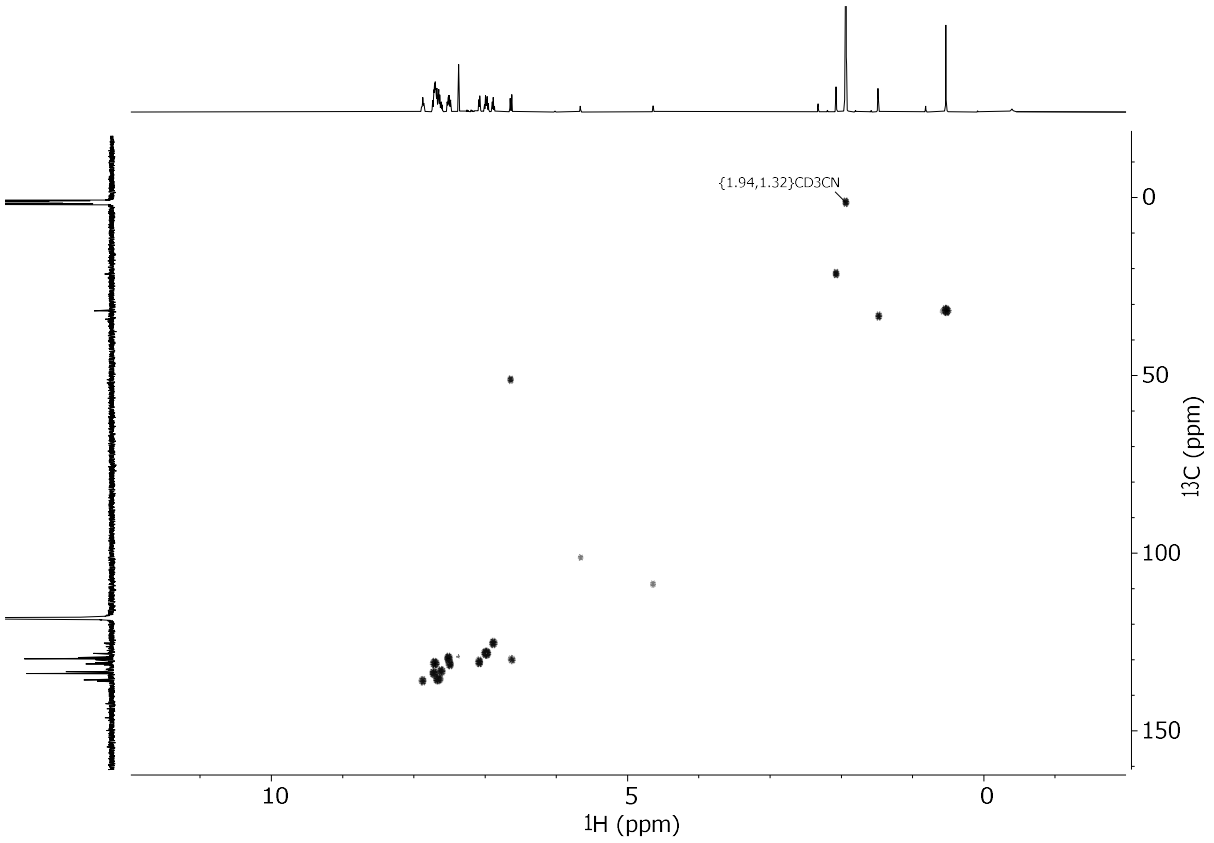


Figure S 109 *^{13}C-^{1}H HSQC NMR spectrum of **3**-$(PPh_4)_2$ in MeCN-d_3 at 298 K.*

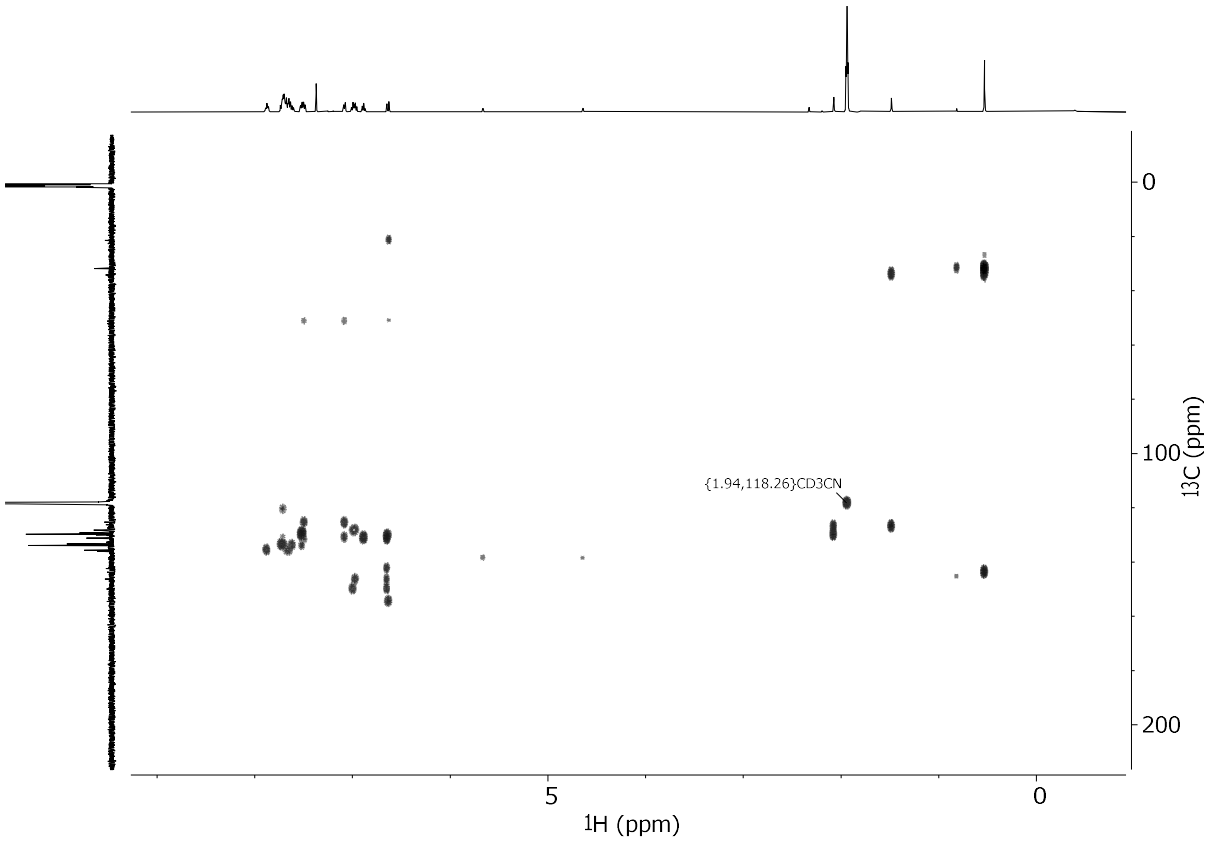


Figure S 110 *^{13}C-^{1}H HMBC NMR spectrum of **3**-$(PPh_4)_2$ in MeCN-d_3 at 298 K.*

[TMA][(^{Ar*}NON)CaCl(thf)$_x$] (4-TMA)

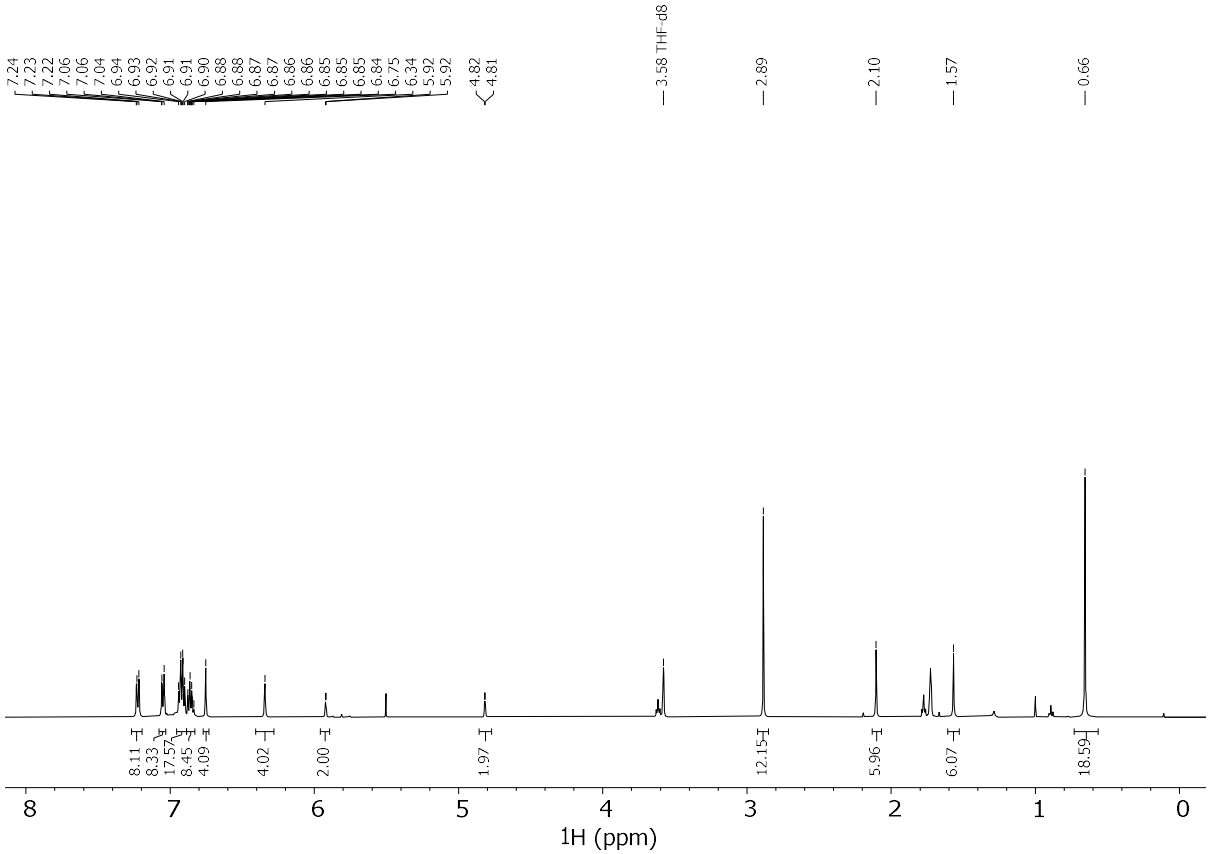


Figure S 111 *^{1}H NMR spectrum of an in-situ reaction forming **4**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the dichloride, **4**-TMA cannot be purified.*

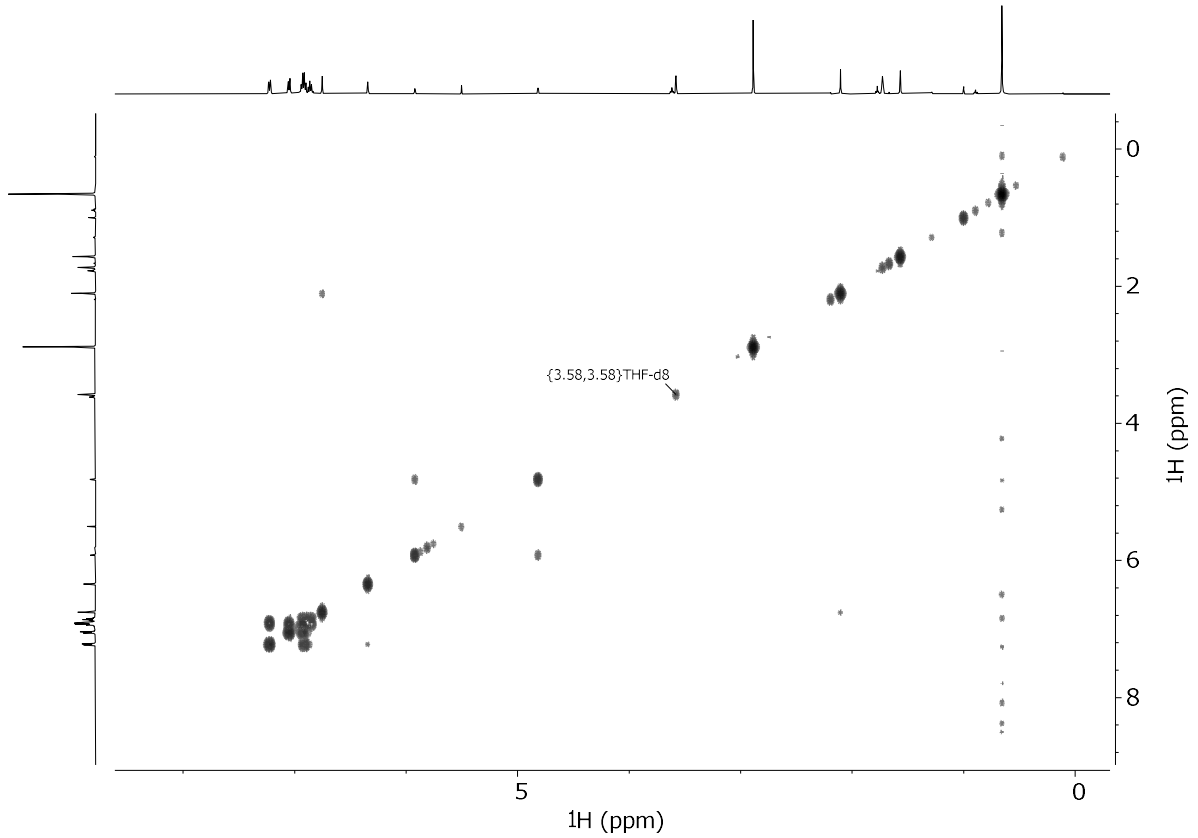


Figure S 112 *^{1}H-^{1}H COSY NMR spectrum of an in-situ reaction forming **4**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the dichloride, **4**-TMA cannot be purified.*

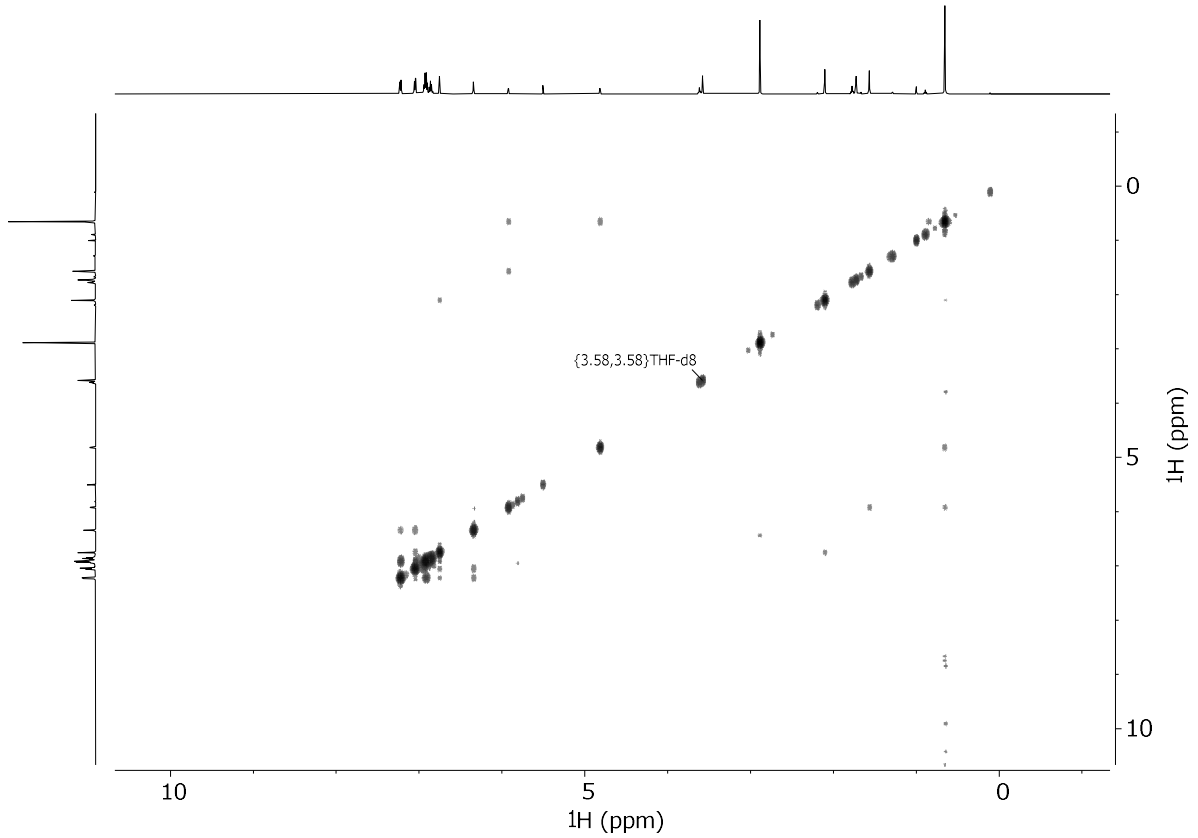


Figure S 113 *^{1}H-^{1}H NOESY NMR spectrum of an in-situ reaction forming **4**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the dichloride, **4**-TMA cannot be purified.*

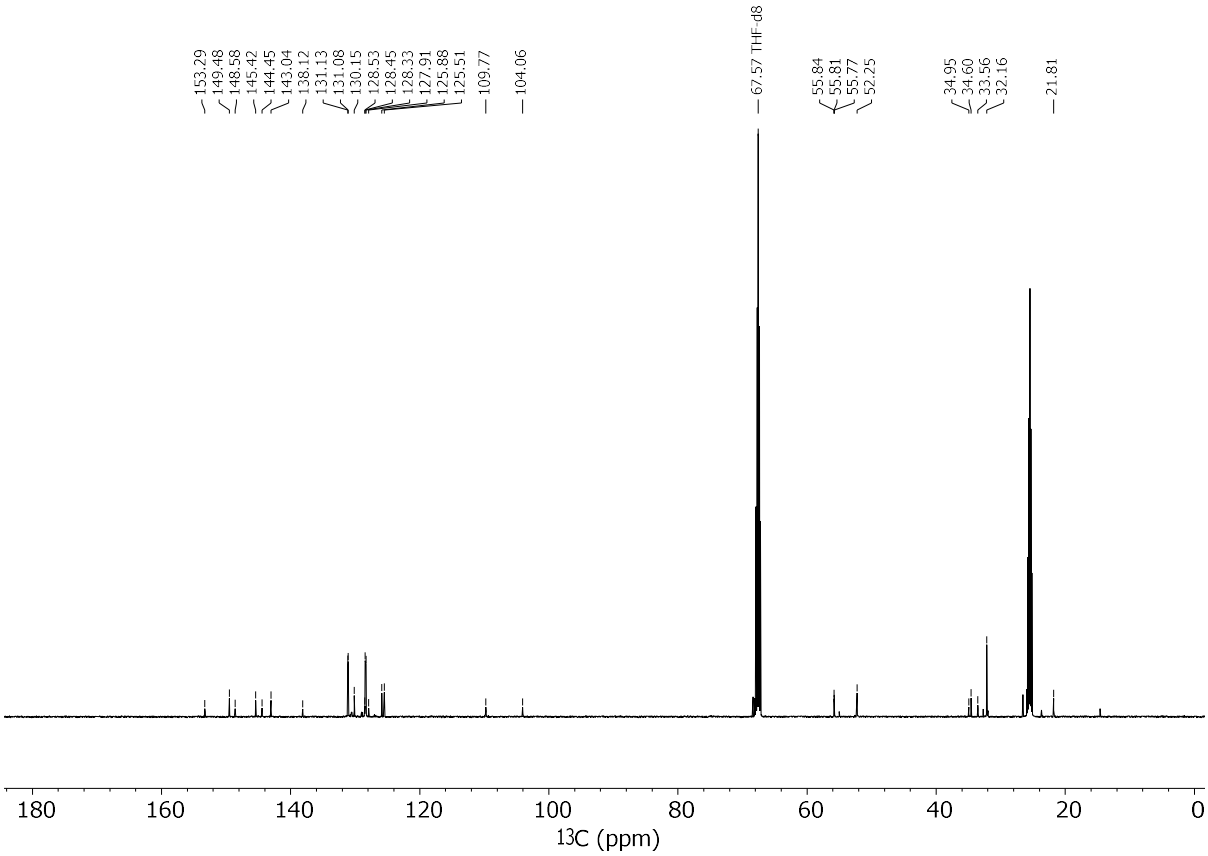


Figure S 114 *$^{13}C\{^{1}H\}$ NMR spectrum of an in-situ reaction forming **4**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the dichloride, **4**-TMA cannot be purified.*

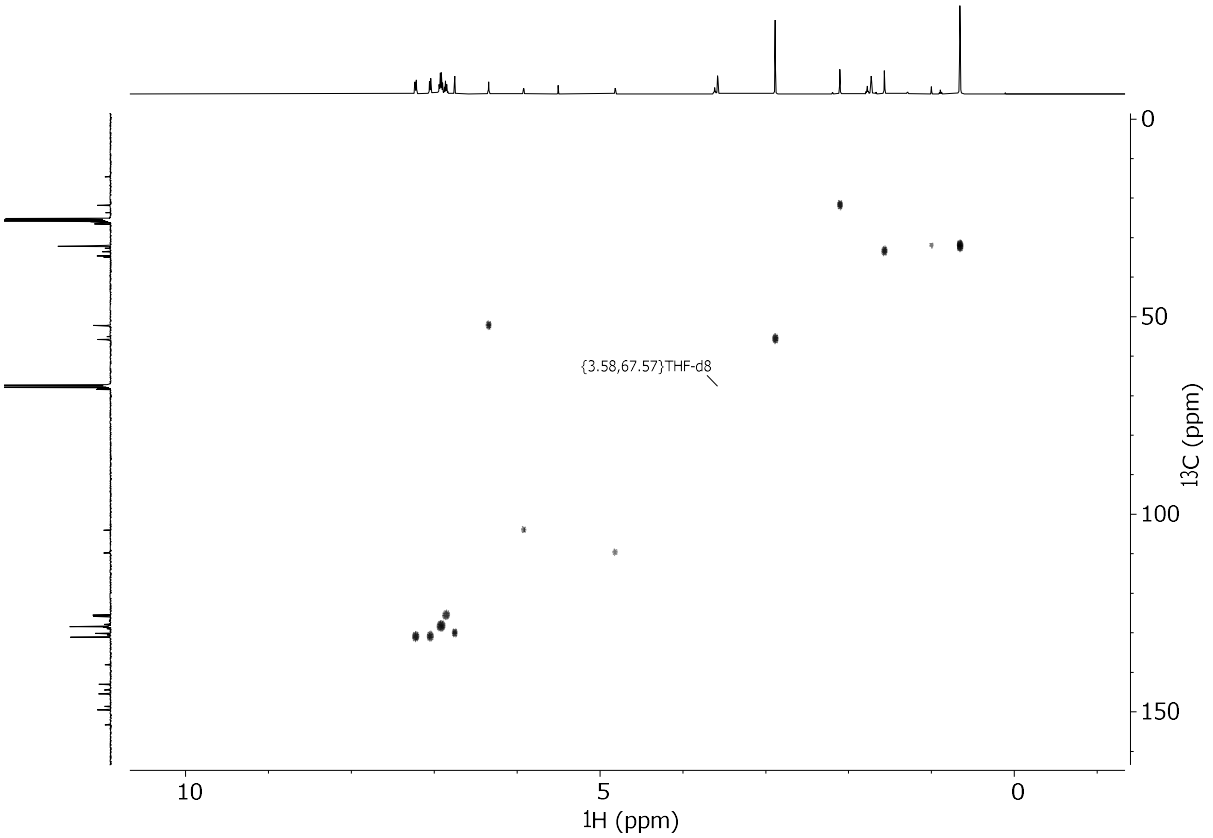


Figure S 115 *^{13}C-^{1}H HSQC NMR spectrum of an in-situ reaction forming **4**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the dichloride, **4**-TMA cannot be purified.*

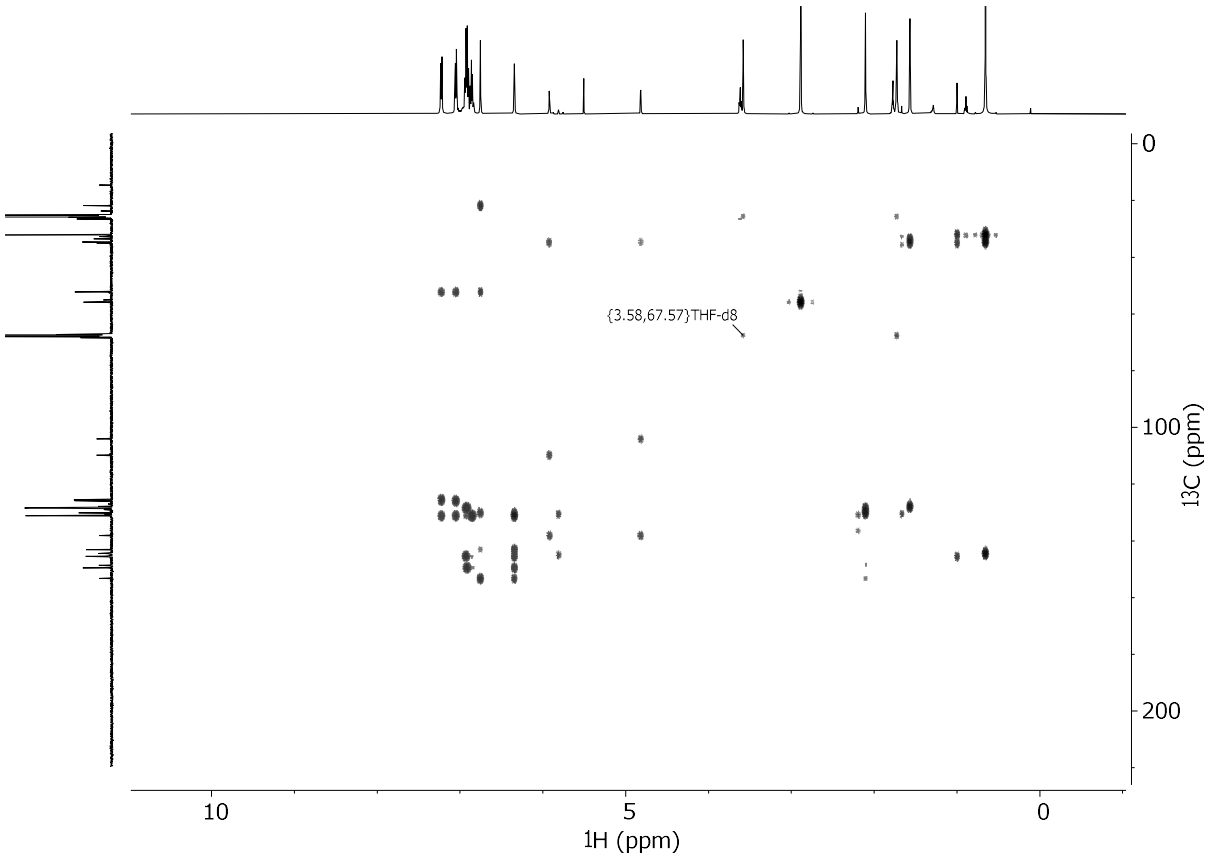


Figure S 116 *^{13}C-^{1}H HMBC NMR spectrum of an in-situ reaction forming **4**-TMA in thf-d_8 at 298 K. Due to all crystallizations resulting in the dichloride, **4**-TMA cannot be purified.*

[PPh_4][(^{Ar*}NON)CaCl(thf)] (4-PPh_4)

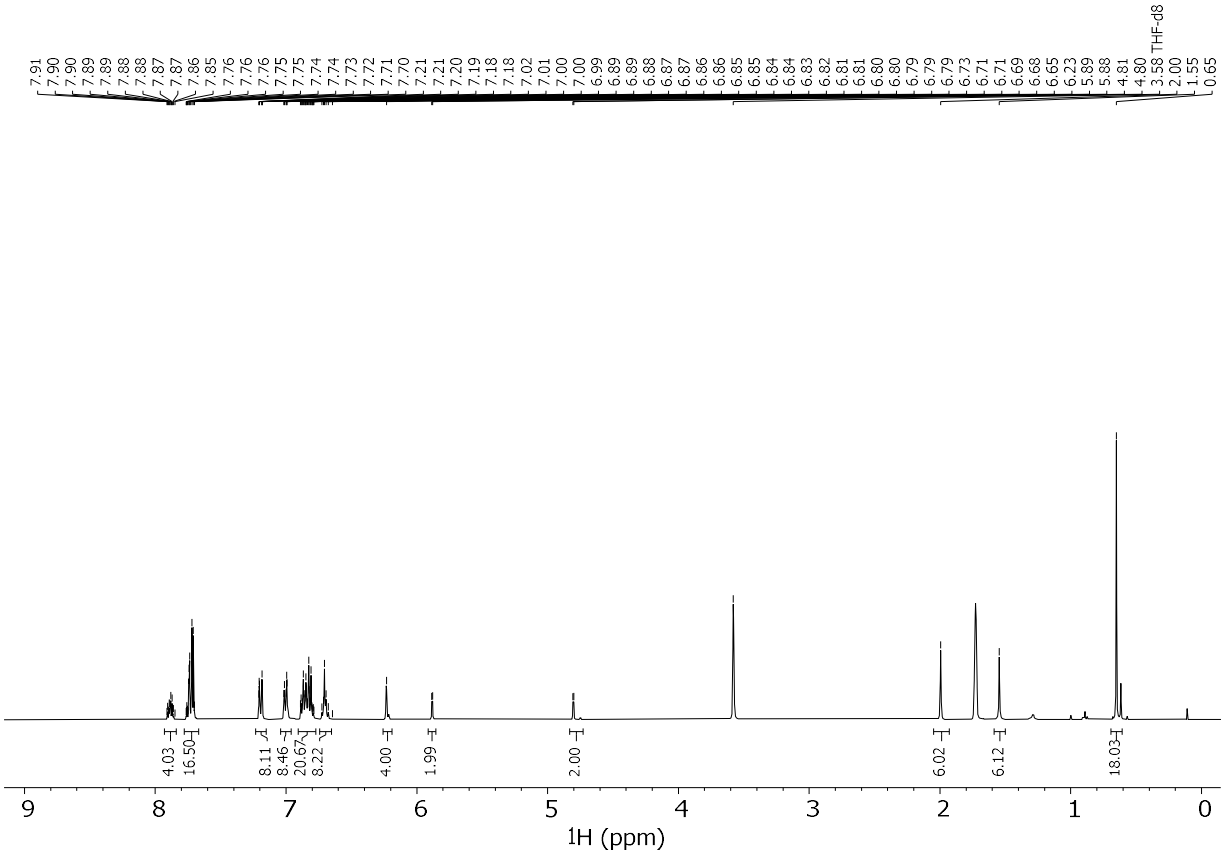


Figure S 117 *^{1}H NMR spectrum of **4**-PPh_4 in thf-d_8 at 298 K.*

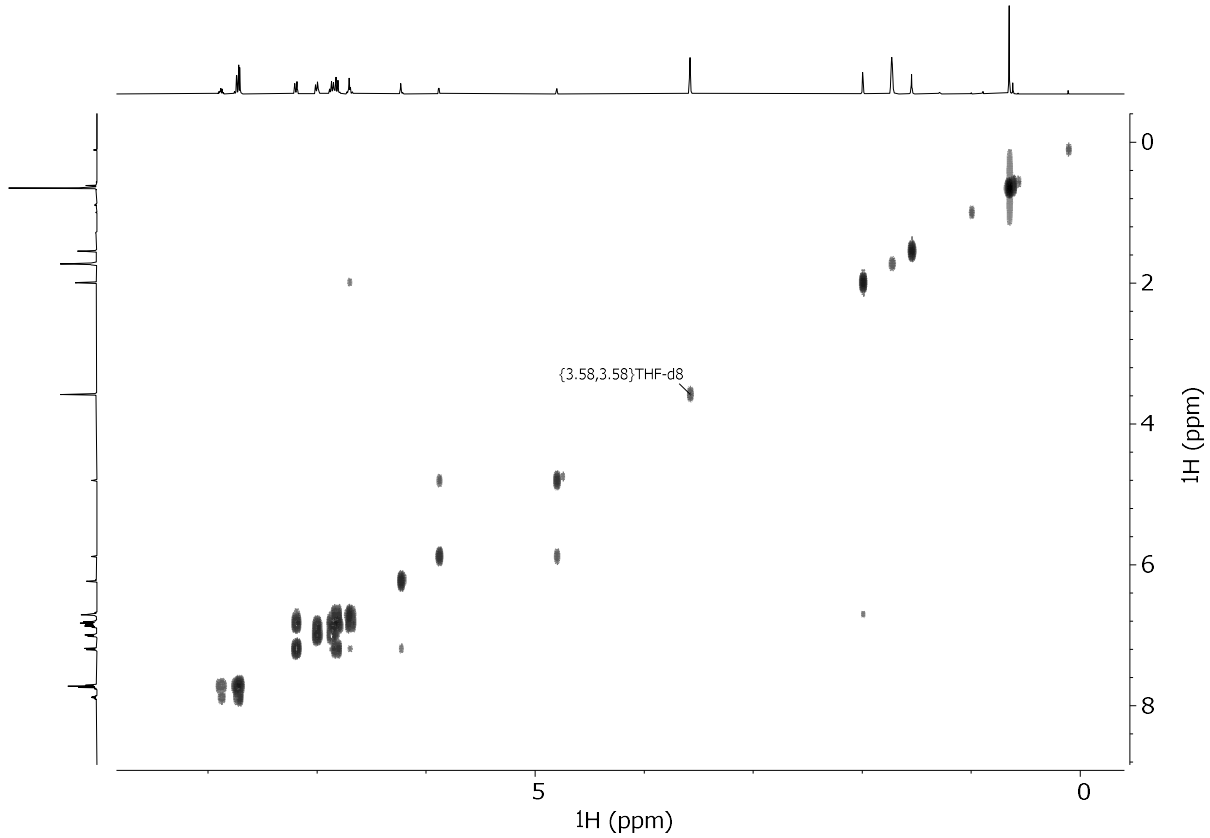


Figure S 118 *^{1}H-^{1}H COSY NMR spectrum of **4**-PPh_4 in thf-d_8 at 298 K.*

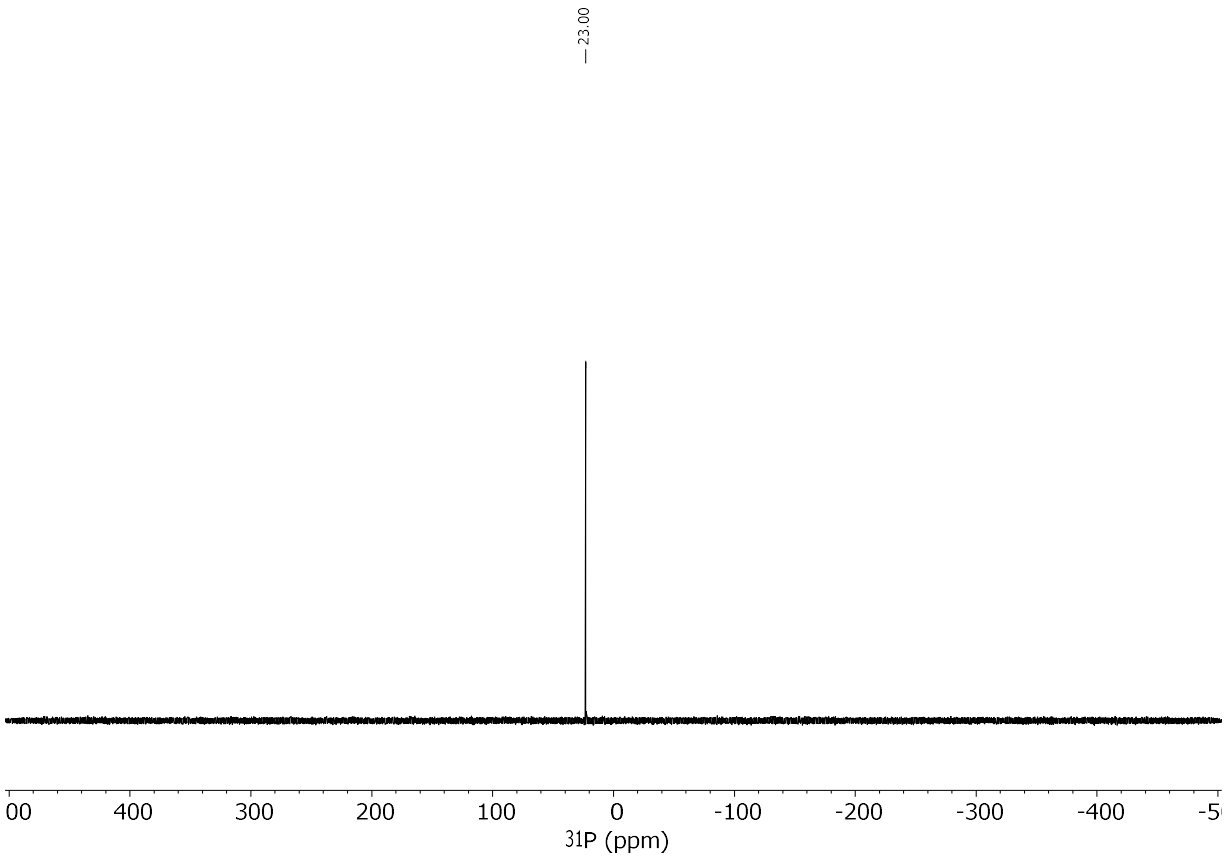


Figure S 119 *^{31}P NMR spectrum of **4**-PPh_4 in thf-d_8 at 298 K.*

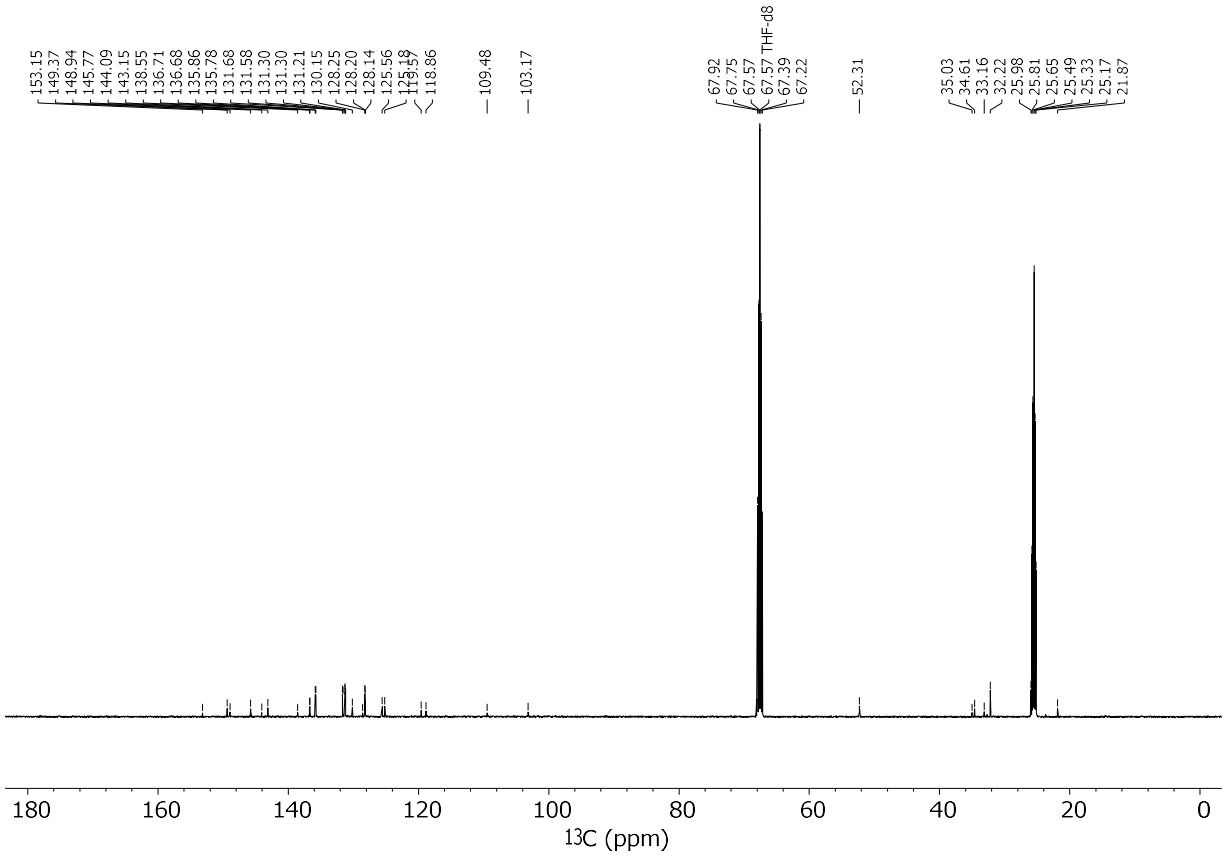


Figure S 120 *$^{13}C\{^{1}H\}$ NMR spectrum of **4**-PPh_4 in thf-d_8 at 298 K.*

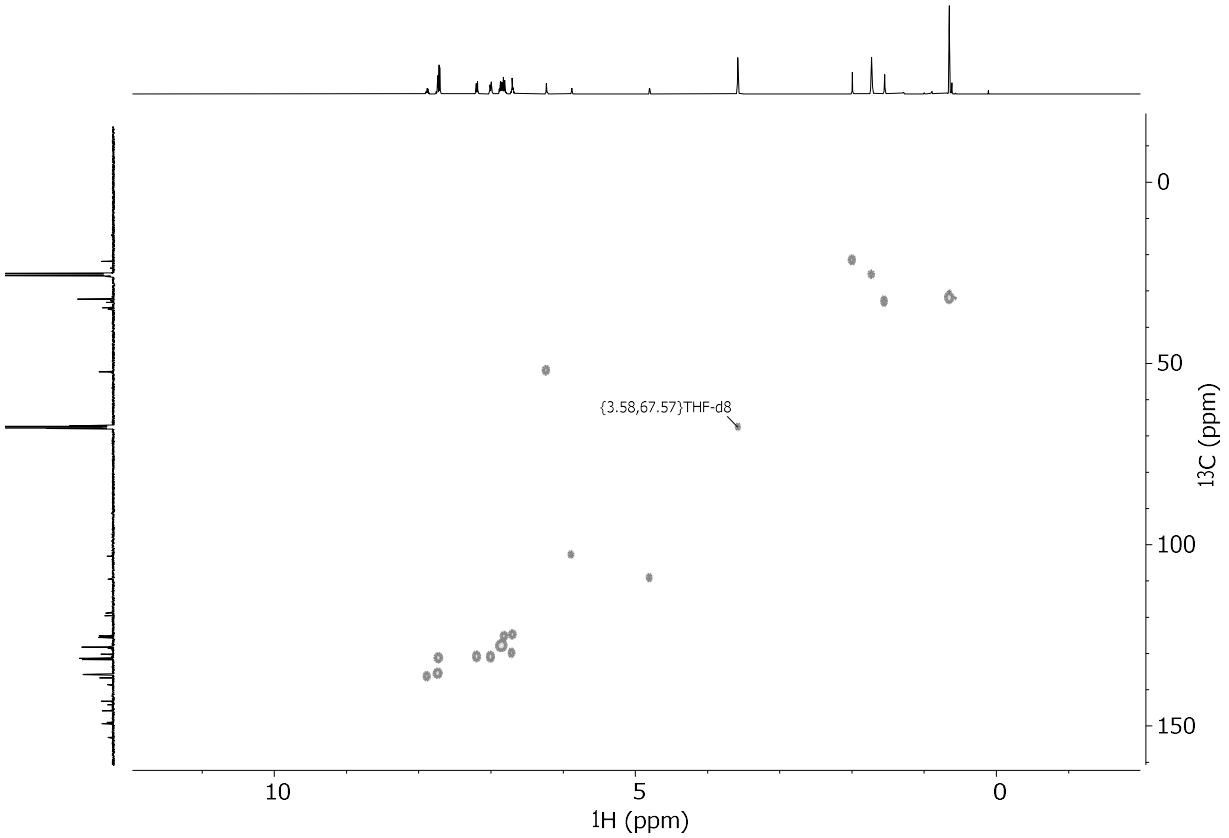


Figure S 121 *^{13}C-^{1}H HSQC NMR spectrum of **4**-PPh_4 in thf-d_8 at 298 K.*

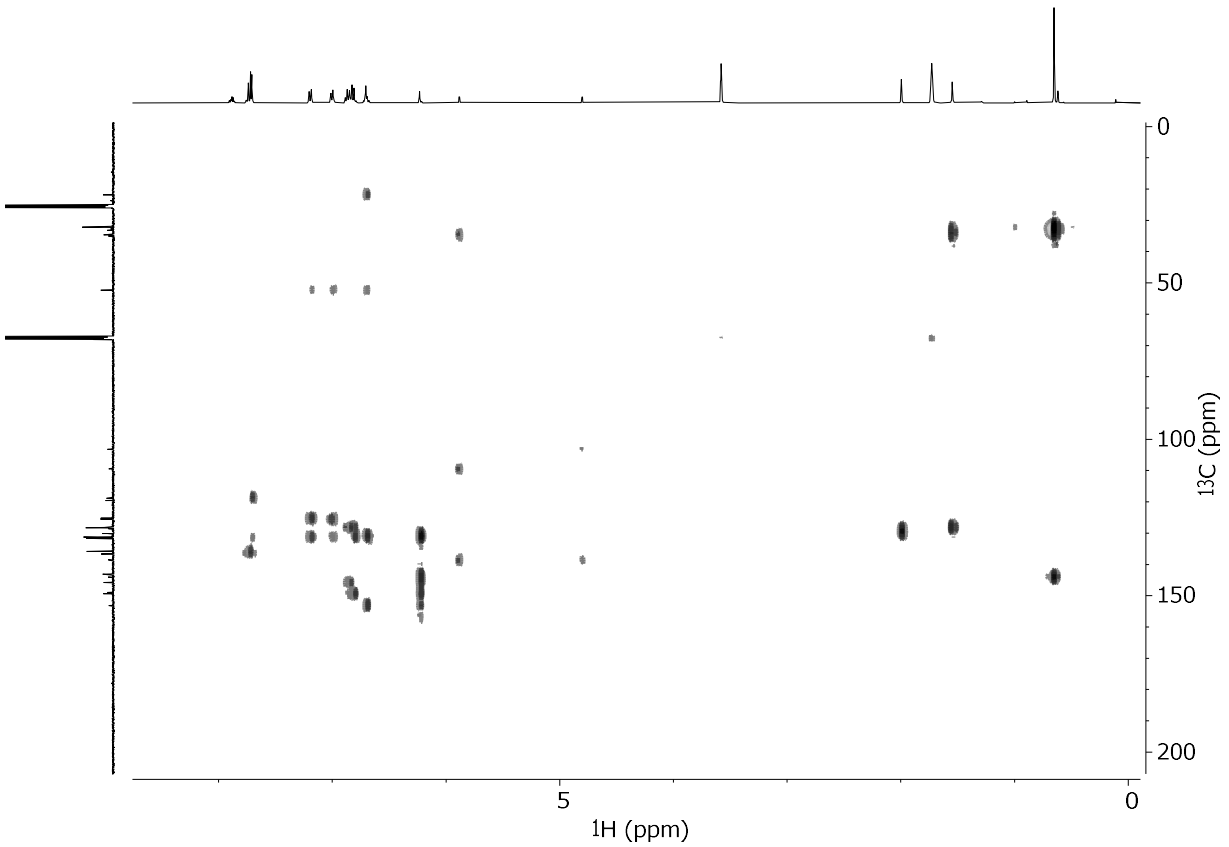


Figure S 122 *^{13}C-^{1}H HMBC NMR spectrum of **4**-PPh_4 in thf-d_8 at 298 K.*

[K(2.2.2-crypt)][(^{Ar*}NON)CaF] (6-KCrypt)

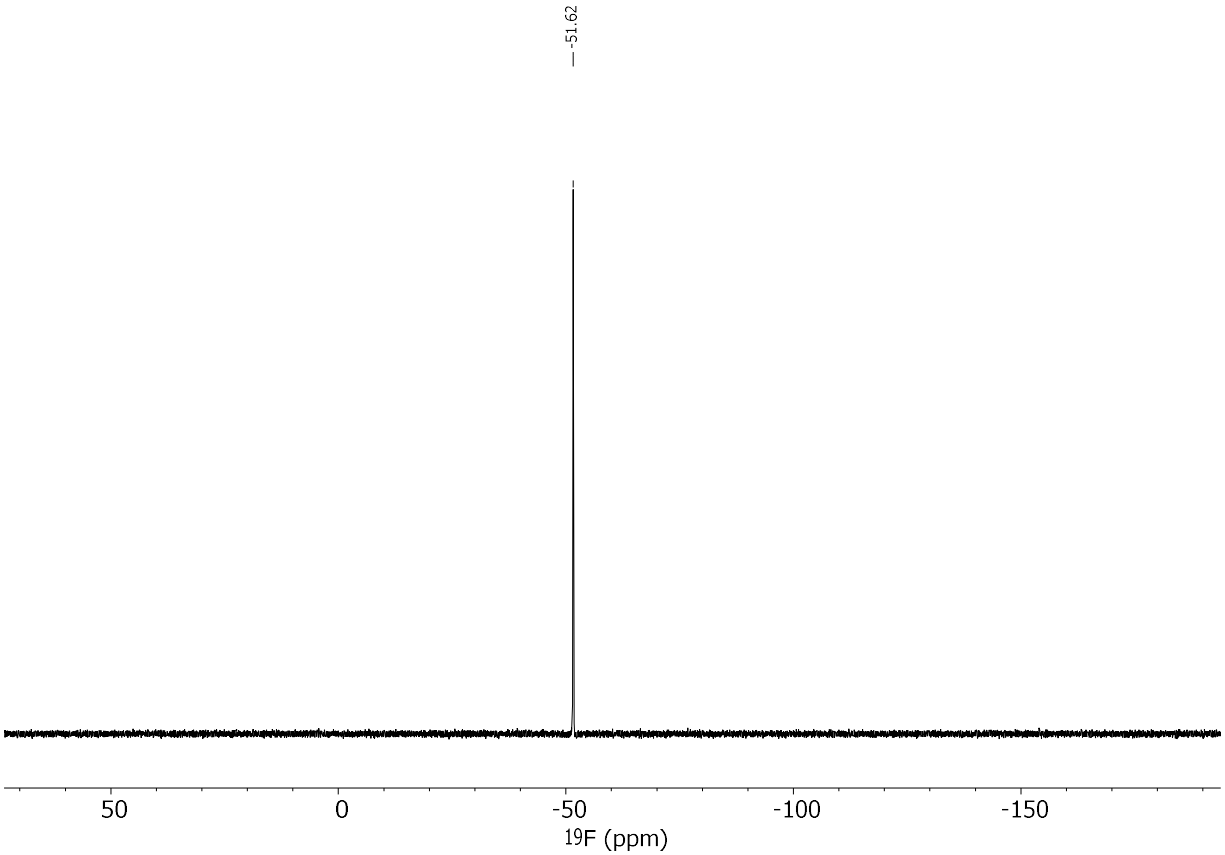


Figure S 123 *^{19}F NMR spectrum of **6**-KCrypt in 2-MeThf at 298 K.*

Biphenyl-4-d_2-methanol

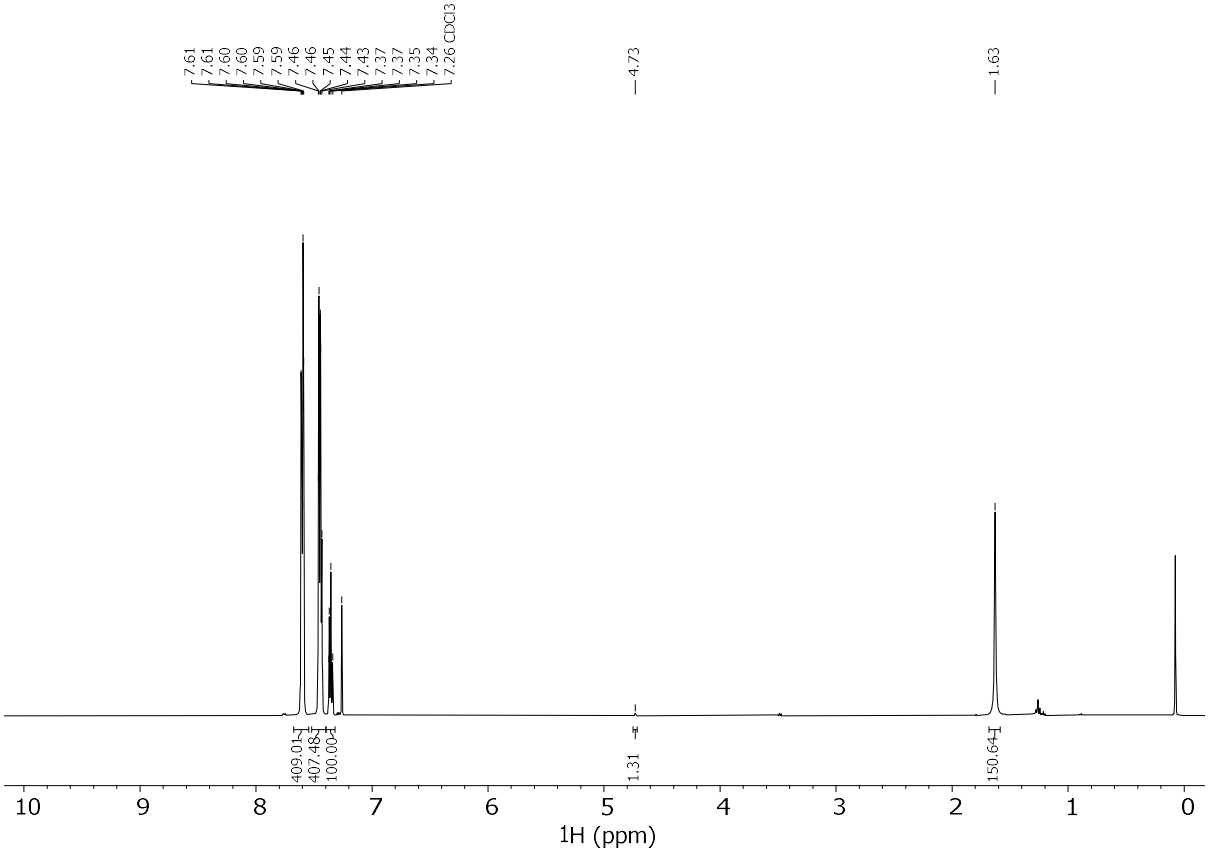


Figure S 124 *^{1}H NMR quantitative spectrum of biphenyl-4-d_2-methanol in $CDCl_3$ at 298 K.*

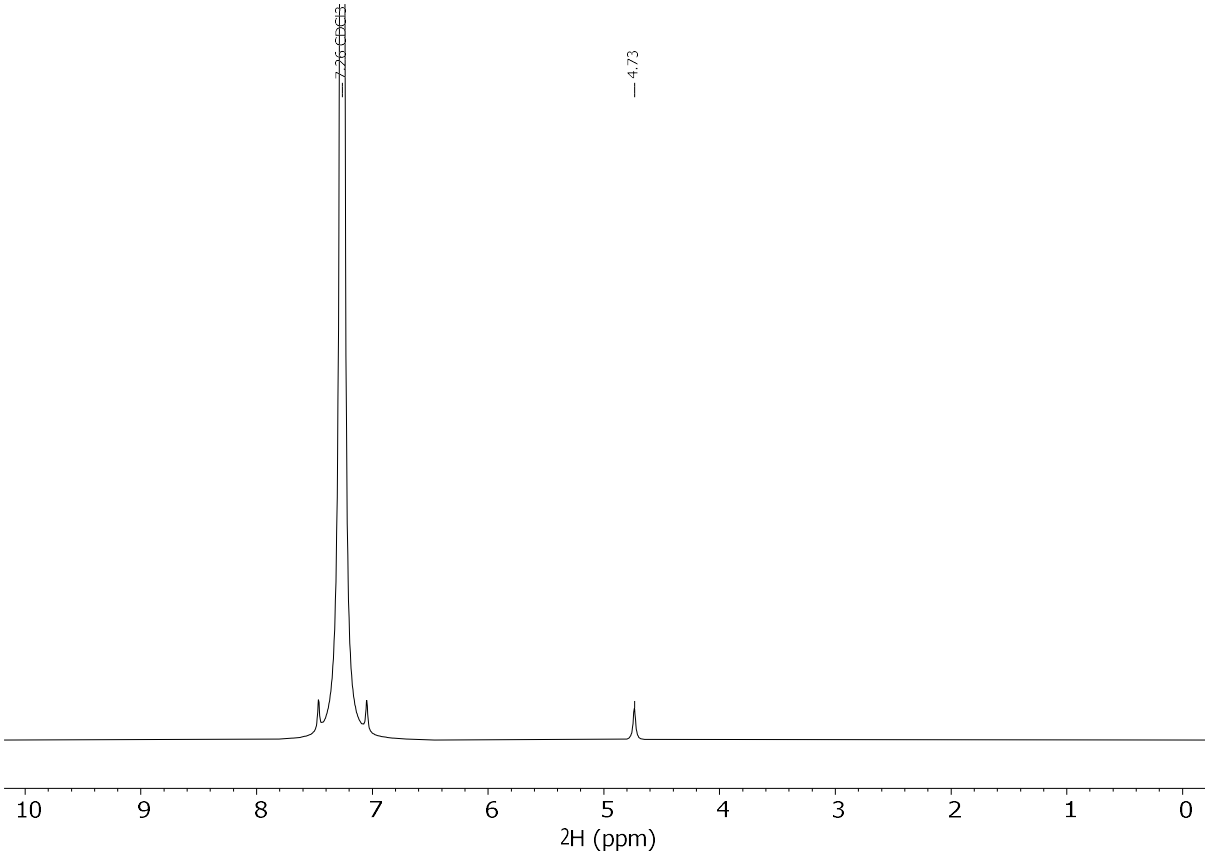


Figure S 125 *^{2}D NMR spectrum of biphenyl-4-d_2-methanol in $CDCl_3$ at 298 K.*

4-(bromo-d_2-methyl)-biphenyl

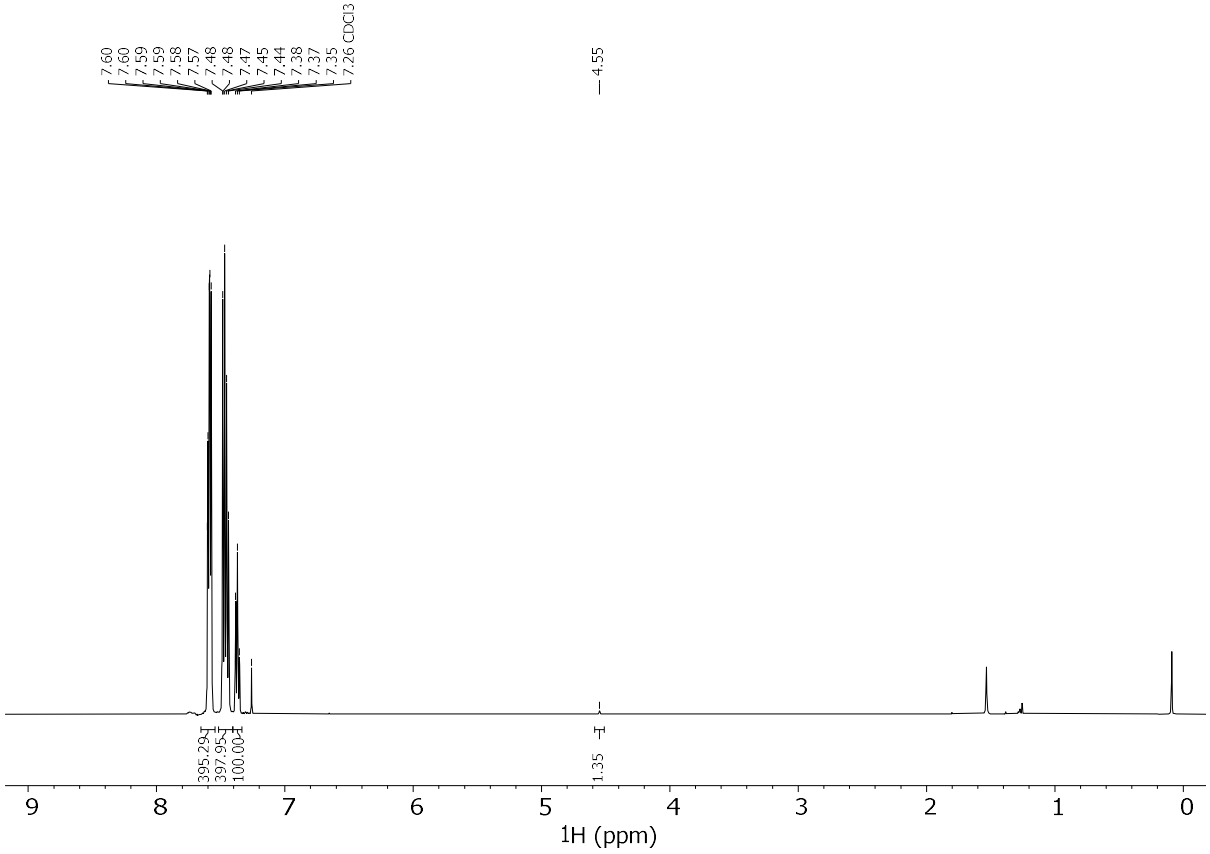


Figure S 126 *^{1}H NMR quantitative spectrum of 4-(bromo-d_2-methyl)-biphenyl in $CDCl_3$ at 298 K.*

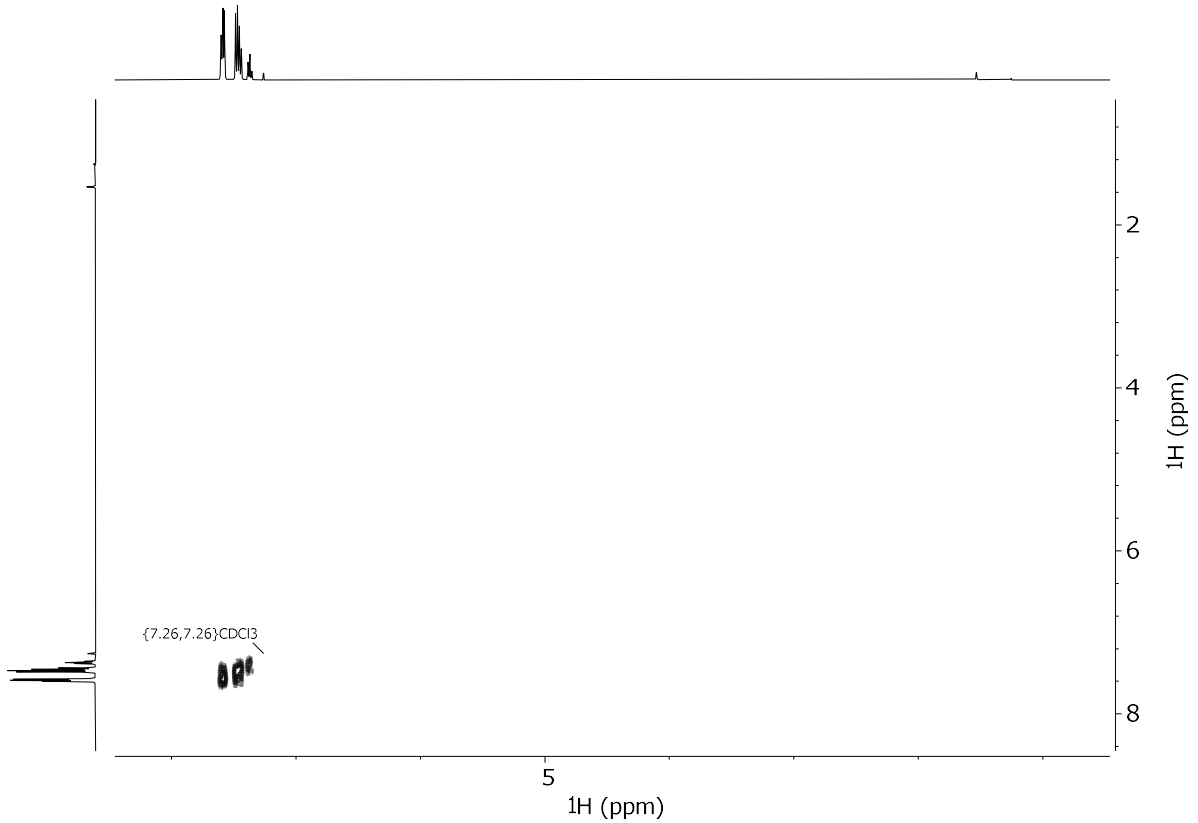


Figure S 127 *^{1}H-^{1}H COSY NMR spectrum of 4-(bromo-d_2-methyl)-biphenyl in $CDCl_3$ at 298 K.*

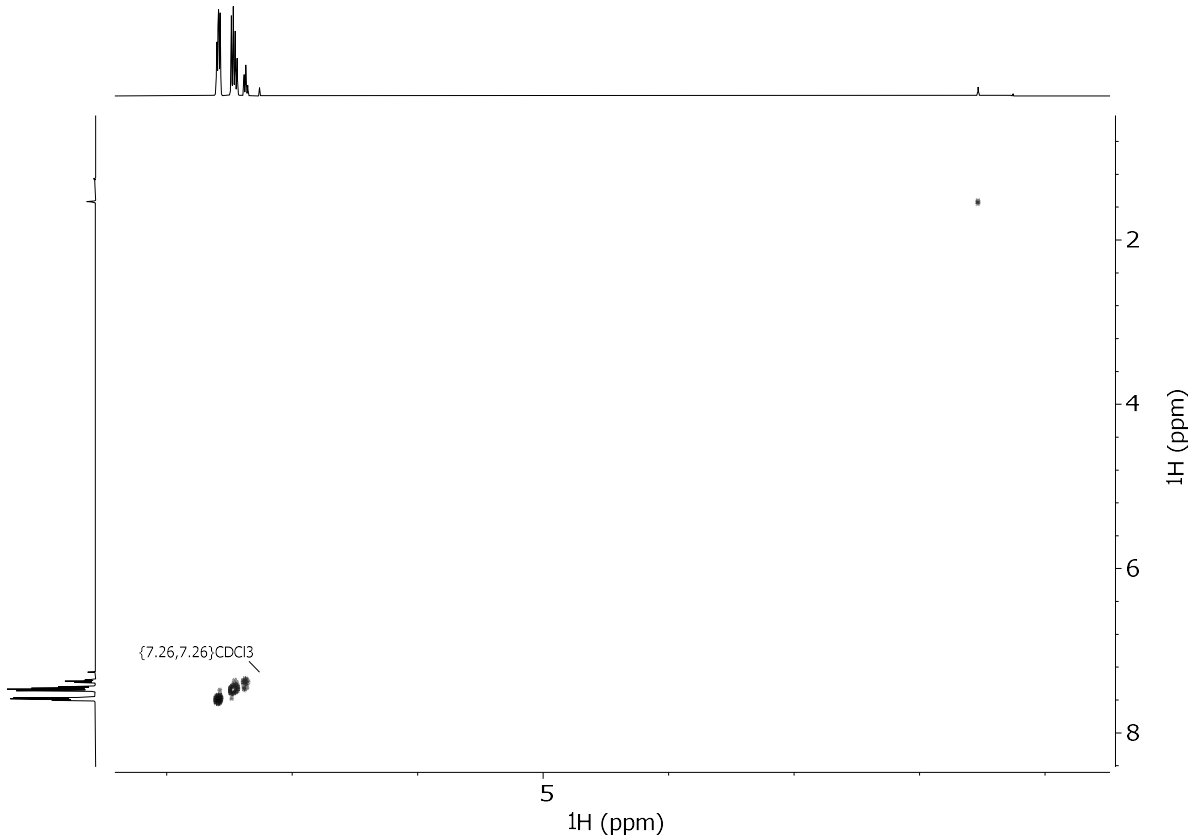


Figure S 128 *^{1}H-^{1}H NOESY NMR spectrum of 4-(bromo-d_2-methyl)-biphenyl in $CDCl_3$ at 298 K.*

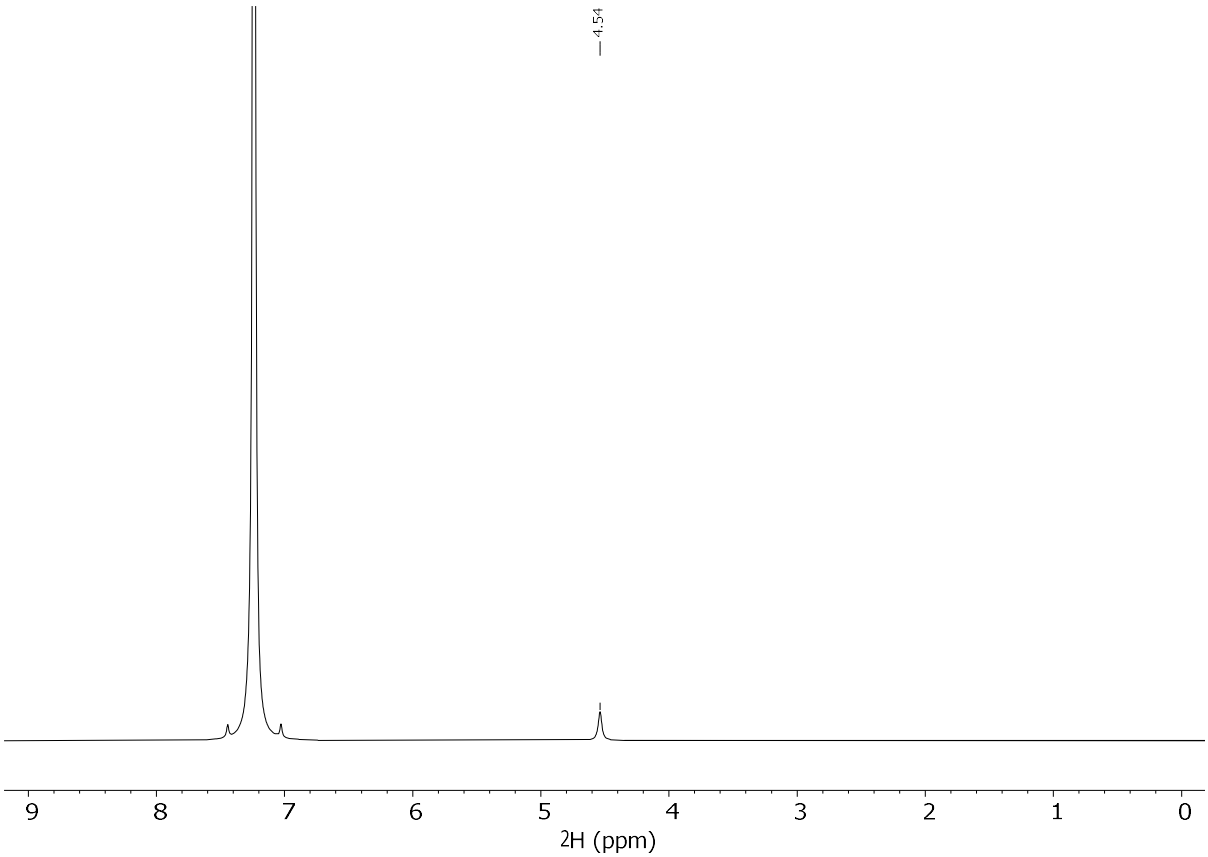


Figure S 129 *^{2}D NMR spectrum of 4-(bromo-d_2-methyl)-biphenyl in $CDCl_3$ at 298 K.*

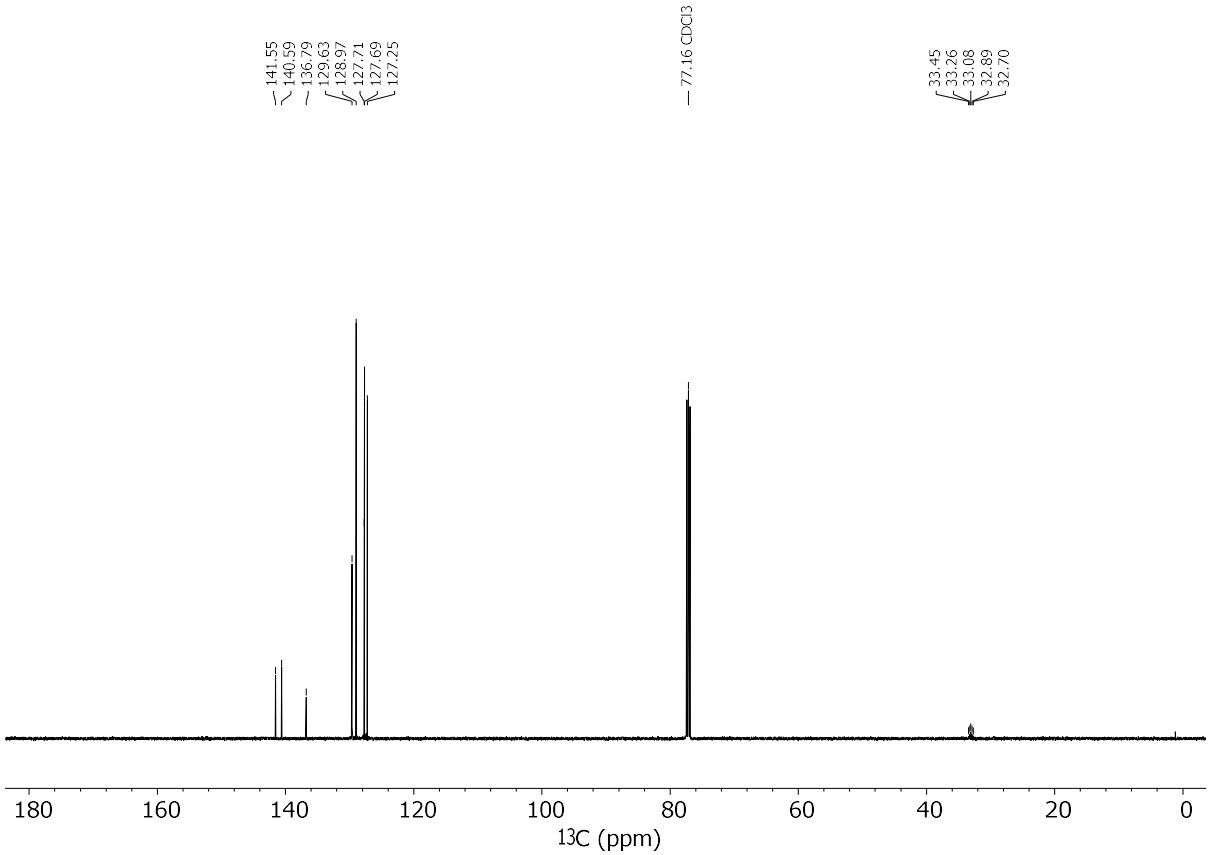


Figure S 130 *$^{13}C\{^{1}H\}$ NMR spectrum of 4-(bromo-d_2-methyl)-biphenyl in $CDCl_3$ at 298 K.*

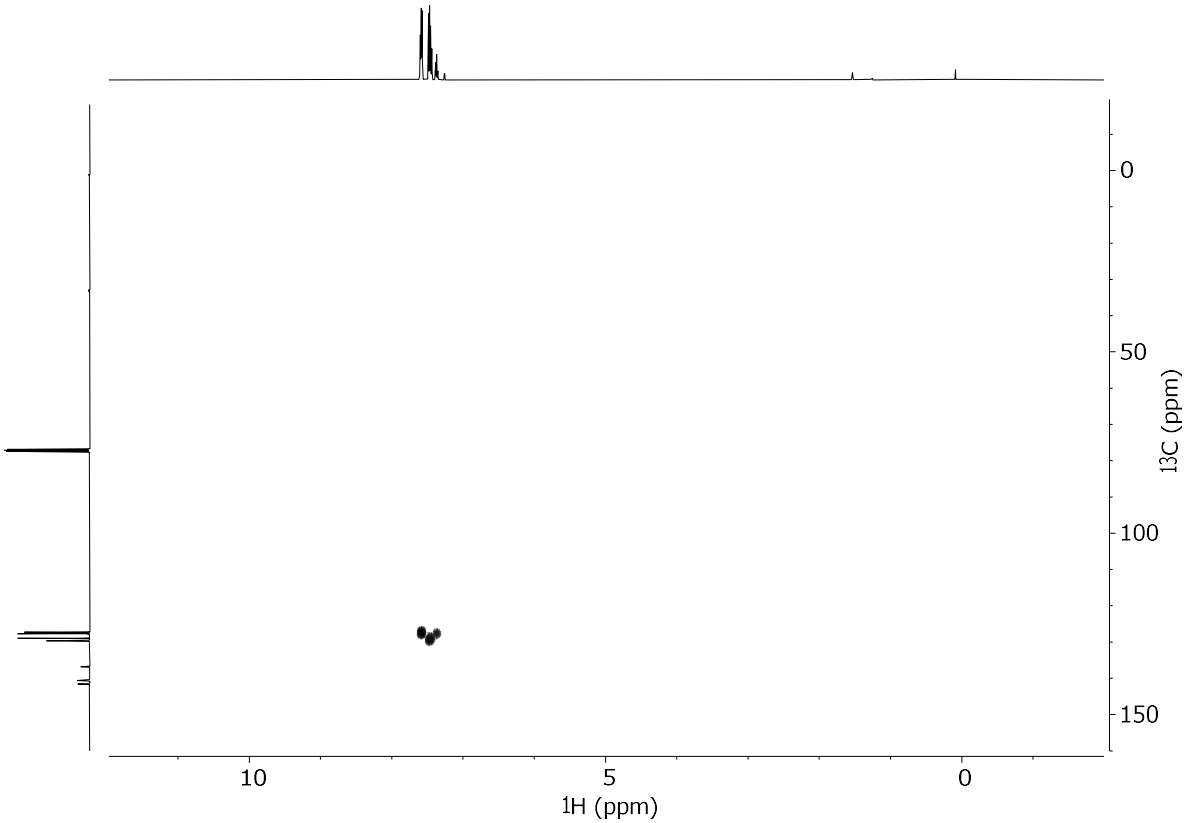


Figure S 131 *^{13}C-^{1}H HSQC NMR spectrum of 4-(bromo-d_2-methyl)-biphenyl in $CDCl_3$ at 298 K.*

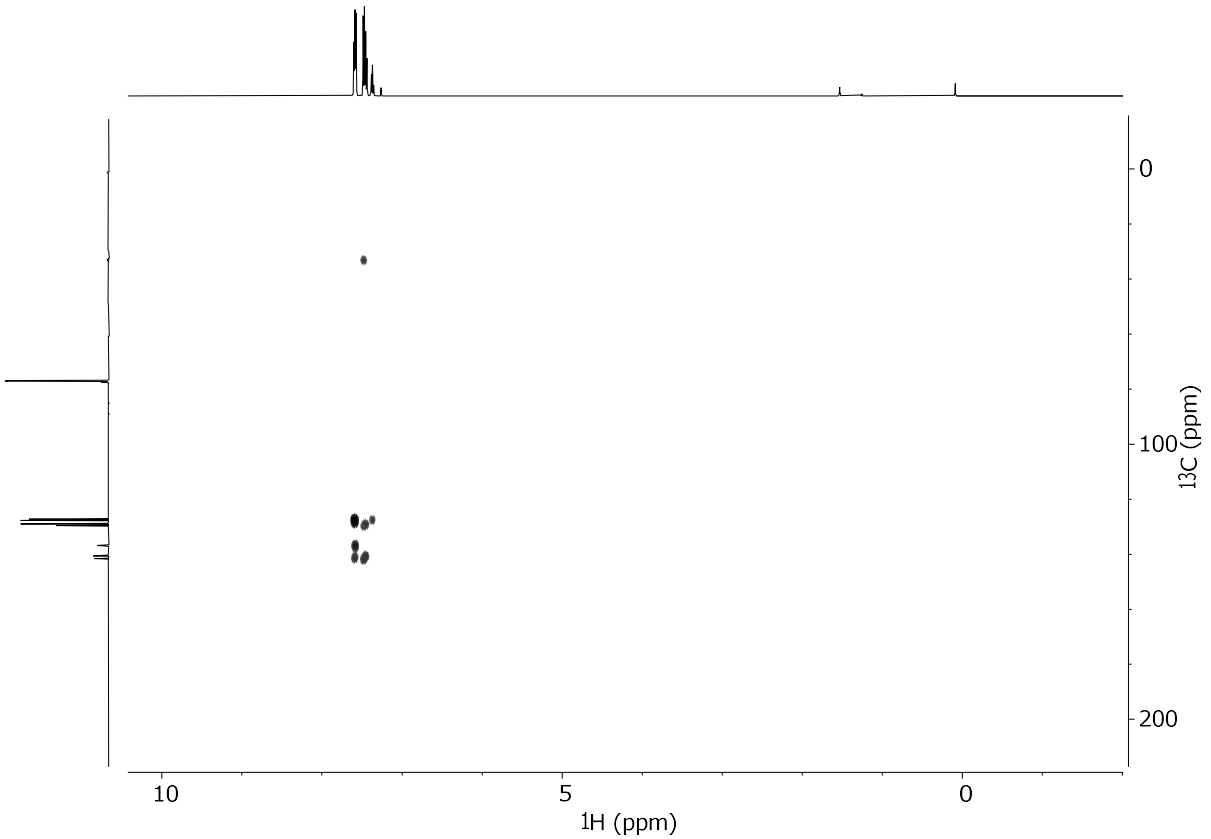


Figure S 132 *^{13}C-^{1}H HMBC NMR spectrum of 4-(bromo-d_2-methyl)-biphenyl in $CDCl_3$ at 298 K.*

4. X-ray crystallographic data

Table S1. *Crystal data and refinement details for the crystal structure analysis of* ***1****-□,* ***1****-thf and* ***1****-thf₂.*

	(^{Ar*}NON)Ca	**(^{Ar*}NON)Ca(thf)**	**(^{Ar*}NON)Ca(thf)₂**
	1-□	**1-thf**	**1-thf₂**
formula	C89 H82 Ca N2 O + 3 C6H8 + C6H14	C93 H90 Ca N2 O2 + C6H14	C97 H98 Ca N2 O3 + 3.5 C4H8O
formula weight / g·mol^{-1}	1562.18	1393.92	1632.21
crystal system	monoclinic	monoclinic	triclinic
space group	$P2_1/n$	$P2_1/n$	$P\bar{1}$
a / Å *b* / Å *c* / Å	16.1890(2) 33.6980(3) 17.2089(2)	14.5998(1) 17.3963(1) 31.3161(1)	15.4906(3) 18.1488(3) 18.8195(5)
α / ° β / ° γ / °	90 108.984(1) 90	90 99.895(1) 90	82.077(2) 70.002(2) 68.742(2)
volume / Å^3 *Z* ρ_{calc} / g·cm^{-3}	8877.5(2) 4 1.169	7835.4(1) 4 1.182	4633.0(2) 2 1.170
radiation (Å)	Cu Kα (1.54184)	Cu Kα (1.54184)	Cu Kα (1.54184)
temperature / K	100.0(1)	150.0(2)	200.0(1)
μ / mm^{-1}	1.000	1.083	1.022
crystal size / mm^3	0.29 × 0.07 × 0.02	0.14 × 0.13 × 0.10	0.11 × 0.05 × 0.04
F(000)	3360	2992	1756
2θ range / °	5.244 - 150.098	5.730 - 152.534	4.998 - 145.626
reflection collected	292302	191855	148599
independent reflections R_{int}	18074 0.1176	16360 0.0373	17794 0.0367
data / restraints / parameters	18074 / 0 / 848	16360 / 171 / 1007	17794 / 156 / 987
[a] goodness-of-fit on F^2	1.064	1.060	1.057
[b,c] final *R* indexes [I≥2σ (I)], R_1 / ωR_2	0.0971 / 0.2773	0.0412 / 0.1097	0.0616 / 0.1918
final *R* indexes [all data]	0.1039 / 0.2815	0.0464 / 0.1141	0.0764 / 0.2018
max. peak / hole in e·Å^{-3}	0.97 / -0.57	0.85 / -0.85	0.54 / -0.36
CCDC reference[d]	2488581	2488583	2488579

[a] $S = \{\sum[\omega(F_o^2-F_c^2)^2]/(n-p)\}^{0.5}$; n = no. of reflections; p = no. of parameters. [b] $R_1 = \sum||F_0|-|F_c||/\sum|F_0|$. [c] $\omega R_2 = \{\sum[\omega(F_o^2-F_c^2)^2]/\sum[\omega(F_o^2)^2]\}^{0.5}$. [d] data are available free of charge via "www.ccdc.cam.ac.uk/data_request/cif".

Table S2. *Crystal data and refinement details for the crystal structure analysis of* ***2****-PPh₄,* ***3****-TMA₂ and* ***3****-(PPh₄)₂.*

	[PPh₄][(^{Ar*}NON)CaF(thf)] **2-PPh₄**	**[TMA]₂[(^{Ar*}NON)CaF₂]** **3-TMA₂**	**[PPh₄]₂[(^{Ar*}NON)CaF₂]** **3-(PPh₄)₂**
formula	C117 H110 Ca F N2 O2 P + 5 C4H8O	C97 H106 Ca F2 N4 O + 3.5 C4H8O	C137 H122 Ca F2 N2 O P + 5 C6H4F2
formula weight / g·mol^{-1}	2026.63	1674.29	2522.84
crystal system	triclinic	monoclinic	monoclinic
space group	$P\bar{1}$	$P2_1/n$	$P2_1/n$
a / Å *b* / Å *c* / Å	15.2188(1) 19.2673(1) 20.4607(1)	16.9867(1) 47.4876(2) 23.8832(1)	17.3555(2) 41.9926(4) 18.2528(2)
α / ° β / ° γ / °	75.307(1) 87.628(1) 86.155(1)	90 101.429(1) 90	90 97.617(1) 90
volume / Å^3 *Z* ρ_{calc} / g·cm^{-3}	5788.5(1) 2 1.163	18883.6(1) 8 1.178	13185.3(2) 4 1.271
radiation (Å)	Cu Kα (1.54184)	Cu Kα (1.54184)	Cu Kα (1.54184)
temperature / K	100.0(1)	100.0(1)	100.0(1)
μ / mm^{-1}	1.056	1.035	1.238
crystal size / mm^3	0.15 × 0.11 × 0.09	0.12 × 0.10 × 0.04	0.26 × 0.03 × 0.01
F(000)	2172	7216	5296
2θ range / °	4.466 - 152.168	3.722 - 152.050	4.208 - 145.184
reflection collected	272800	546400	116507
independent reflections R_{int}	23765 0.0377	39068 0.0569	24988 0.0462
data / restraints / parameters	23765 / 86 / 1176	39068 / 186 / 2048	24988 / 490 / 1725
[a] goodness-of-fit on F^2	1.043	1.069	1.037
[b,c] final *R* indexes [I≥2σ (I)], R_1 / ωR_2	0.0645 / 0.1936	0.0963 / 0.2705	0.0518 / 0.1399
final *R* indexes [all data]	0.0697 / 0.1974	0.0994 / 0.2722	0.067 / 0.1496
max. peak / hole in e·Å^{-3}	0.65 / -0.55	0.66 / -0.62	0.83 / -0.69
CCDC reference[d]	2488584	2488582	2488576

[a] $S = \{\sum[\omega(F_o^2-F_c^2)^2]/(n-p)\}^{0.5}$; n = no. of reflections; p = no. of parameters. [b] $R_1 = \sum||F_0|-|F_c||/\sum|F_0|$. [c] $\omega R_2 = \{\sum[\omega(F_o^2-F_c^2)^2]/\sum[\omega(F_o^2)^2]\}^{0.5}$. [d] data are available free of charge via "www.ccdc.cam.ac.uk/data_request/cif".

Table S3. *Crystal data and refinement details for the crystal structure analysis of* ***4****-PPh₄,* ***5****-TMA₂ and* ***7****-TMA₂.*

	[PPh₄] [(Ar*NON)CaCl(thf)]	**[TMA]₂ [(Ar*NON)CaCl₂]**	**[TMA]₂ [(Ar*NON)CaFCl]**
	4-PPh₄	**5-TMA₂**	**7-TMA₂**
formula	C117 H110 Ca Cl N2 O2 P + C4H8O	C97 H106 Ca Cl2 N4 O + 4 C4H8O	C97 H106 Ca Cl F N4 O + 4 C4H8O
formula weight / g·mol^{-1}	1754.67	1454.83	1726.80
crystal system	triclinic	monoclinic	orthorhombic
space group	$P\bar{1}$	$P2_1/c$	*Cmce*
a / Å *b* / Å *c* / Å	15.2598(1) 15.8321(1) 21.4083(2)	20.8755(4) 15.1966(2) 31.1765(4)	29.5825(4) 23.9143(3) 27.8627(4)
α / ° β / ° γ / °	90.016(1) 110.159(1) 92.486(1)	90 90.854(1) 90	90 90 90
volume / Å^3 *Z* ρ_{calc} / g·cm^{-3}	4850.1(1) 2 1.202	9889.2(3) 4 0.977	19711.3(5) 8 1.164
radiation (Å)	Cu Kα (1.54184)	Cu Kα (1.54184)	Cu Kα (1.54184)
temperature / K	100.0(1)	100.0(1)	100.0(1)
μ / mm^{-1}	1.387	1.358	1.238
crystal size / mm^3	0.17 × 0.09 × 0.06	0.11 × 0.07 × 0.02	0.08 × 0.04 × 0.02
F(000)	1868	3112	7440
2θ range / °	4.398 to 149.008	4.234 to 145.67	5.714 - 152.712
reflection collected	108144	77826	117267
independent reflections R_{int}	19685 0.0323	18672 0.0647	10344 0.0822
data / restraints / parameters	19685 / 186 / 1329	18672 / 663 / 1052	10344 / 144 / 574
[a] goodness-of-fit on F^2	1.054	1.005	1.036
[b,c] final *R* indexes [I≥2σ (I)], R_1 / ωR_2	0.0396 / 0.1052	0.0796 / 0.2236	0.0822 / 0.2259
final *R* indexes [all data]	0.0422 / 0.1069	0.1413 / 0.2624	0.0943 / 0.2341
max. peak / hole in e·Å^{-3}	0.75 / -0.51	0.68 / -0.56	1.11 / -0.43
CCDC reference[d]	2488577	2488575	2488586

[a] $S = \{\sum[\omega(F_o^2-F_c^2)^2]/(n-p)\}^{0.5}$; n = no. of reflections; p = no. of parameters. [b] $R_1 = \sum||F_0|-|F_c||/\sum|F_0|$. [c] $\omega R_2 = \{\sum[\omega(F_o^2-F_c^2)^2]/\sum[\omega(F_o^2)^2]\}^{0.5}$. [d] data are available free of charge via "www.ccdc.cam.ac.uk/data_request/cif".

Table S4. *Crystal data and refinement details for the crystal structure analysis of* ***6****-KCrypt,* ***2****-KCrypt, and (*^{Ar*}*NON)H₂.*

	[K(2.2.2-crypt)] [(Ar*NON)CaF]	**[K(2.2.2-crypt)] [(Ar*NON)CaF(thf)]**	**(Ar*NON)H₂**
	6-KCrypt	**2-KCrypt**	
formula	C107 H118 Ca F K N4 O7 + C5H9O	C111 H126 Ca F K N4 O8 + 2 C6H14 + 2 C4H8O	C89 H84 N2 O + C7H8
formula weight / g·mol^{-1}	1755.35	2058.88	1267.63
crystal system	monoclinic	orthorhombic	monoclinic
space group	$P2_1/c$	*Pccn*	$P2_1/c$
a / Å *b* / Å *c* / Å	14.7890(1) 26.4186(1) 25.0492(1)	25.7501(3) 35.1388(5) 26.1957(3)	25.9429(4) 13.2226(2) 22.8099(4)
α / ° β / ° γ / °	90 96.780(1) 90	90 90 90	90 112.256(2) 90
volume / Å^3 *Z* ρ_{calc} / g·cm^{-3}	9718.4(1) 4 1.200	23702.6(5) 8 1.154	7241.6(2) 4 1.163
radiation (Å)	Cu Kα (1.54184)	Cu Kα (1.54184)	Cu Kα (1.54184)
temperature / K	100.0(1)	100.0(1)	100.0(1)
μ / mm^{-1}	1.419	1.243	0.508
crystal size / mm^3	0.24 × 0.15 × 0.12	0.19 × 0.10 × 0.05	0.17 x 0.14 x 0.02
F(000)	3756	8896	2712
2θ range / °	4.880 - 149.008	5.430 - 146.144	3.680 - 151.904
reflection collected	103865	181677	86273
independent reflections R_{int}	19825 0.0373	22432 0.0621	14846 0.0385
data / restraints / parameters	19825 / 1513 / 1396	22432 / 687 / 1066	14846 / 465 / 1039
[a] goodness-of-fit on F^2	1.040	1.587	1.047
[b,c] final *R* indexes [I≥2σ (I)], R_1 / ωR_2	0.0608 / 0.1725	0.1280 / 0.4088	0.0562 / 0.1435
final *R* indexes [all data]	0.0675 / 0.1774	0.1577 / 0.4278	0.0733 / 0.1539
max. peak / hole in e·Å^{-3}	0.44 / -0.51	0.68 / -0.52	0.57 / -0.33
CCDC reference[d]	2488587	2488580	2488578

[a] $S = \{\sum[\omega(F_o^2-F_c^2)^2]/(n-p)\}^{0.5}$; n = no. of reflections; p = no. of parameters. [b] $R_1 = \sum||F_0|-|F_c||/\sum|F_0|$. [c] $\omega R_2 = \{\sum[\omega(F_o^2-F_c^2)^2]/\sum[\omega(F_o^2)^2]\}^{0.5}$. [d] data are available free of charge via "www.ccdc.cam.ac.uk/data_request/cif".

Table S5. *Crystal data and refinement details for the crystal structure analysis of (^{Ar*}NON)K$_2$,* ***8***-PPh$_4$-□*, and* ***8***-PPh$_4$-thf.*

	(^{Ar*}NON)K$_2$	**[PPh$_4$] [(^{Ar*}NON)CaBr]**	**[PPh$_4$] [(^{Ar*}NON)CaBr(thf)]**
		8-PPh$_4$-□	**8-PPh$_4$-thf**
formula	C89 H82 K2 N2 O + C7H8	C113 H102 Br Ca N2 O P + 3 C4H8O	C117 H110 Br Ca N2 O2 P + 3 C4H8O
formula weight / g·mol^{-1}	1365.89	1871.23	2015.44
crystal system	triclinic	monoclinic	monoclinic
space group	$P\bar{1}$	*I*2/a	*I*2/a
a / Å *b* / Å *c* / Å	12.6268(1) 15.4868(1) 21.7568(2)	32.5895(10) 16.3468(5) 37.8763(16)	37.2639(5) 14.7309(2) 40.5196(5)
α / ° β / ° γ / °	106.102(1) 96.343(1) 112.346(1)	90 99.224(3) 90	90 102.1370(10) 90
volume / Å^3 *Z* ρ_{calc} / g·cm^{-3}	3667.3(1) 2 1.237	19917.1(12) 8 1.248	21745.3(5) 8 1.231
radiation (Å)	Cu Kα (1.54184)	Cu Kα (1.54184)	Cu Kα (1.54184)
temperature / K	100.0(1)	100.0(1)	100.0(1)
μ / mm^{-1}	1.535	1.601	1.516
crystal size / mm^3	0.18 × 0.04 × 0.02	0.46 × 0.03 × 0.01	0.21 x 0.17 x 0.01
F(000)	1452	7936	8576
2θ range / °	4.358 - 151.802	4.728 - 133.202	4.462 - 147.956
reflection collected	167727	59394	127163
independent reflections R_{int}	15040 0.0393	17421 0.2492	127163 0.0620
data / restraints / parameters	15040 / 0 / 921	17421 / 2844 / 1169	21442 / 2193 / 1355
[a] goodness-of-fit on F^2	1.097	1.243	1.077
[b,c] final *R* indexes [I≥2σ (I)], R_1 / ωR_2	0.0658 / 0.1789	0.1484 / 0.3947	0.0587 / 0.1593
final *R* indexes [all data]	0.0694 / 0.1810	0.2757 / 0.4476	0.0764 / 0.1708
max. peak / hole in e·Å^{-3}	0.83 / -0.61	1.46 / -1.24	1.19 / -0.99
CCDC reference[d]	2488585	2566165	2566166

[a] $S = \{\sum[\omega(F_o^2-F_c^2)^2]/(n-p)\}^{0.5}$; n = no. of reflections; p = no. of parameters. [b] $R_1 = \sum||F_0|-|F_c||/\sum|F_0|$. [c] $\omega R_2 = \{\sum[\omega(F_o^2-F_c^2)^2]/\sum[\omega(F_o^2)^2]\}^{0.5}$. [d] data are available free of charge via "www.ccdc.cam.ac.uk/data_request/cif".

5. Quantum chemical computational details

General considerations

All calculations were performed with the ORCA (Revision 6.1.0) program package[19,20]. All visualizations and density difference plots were generated using ChimeraX 10.1[21,22].

Geometry optimisation and frequency calculations

Geometry optimisations and frequency calculations were carried out using the r2SCAN-3c composite method[23]. This approach combines the meta-generalized-gradient approximation (mGGA) functional r2SCAN [24], the def2-TZVPPm basis set[23], the D4 dispersion correction[24], and the geometrical counterpoise correction (gCP)[25,26]. The RIJDX approximation[27], together with the def2-mTZVPP/J auxiliary basis[23], was used throughout to accelerate integral evaluation. The Conductor-like Polarizable Continuum Model (CPCM)[28–30] with tetrahydrofuran (THF) as solvent was employed during all optimisations and frequency analyses. All stationary points were confirmed by full frequency analyses: 0 imaginary frequencies identified minima, while 1 imaginary frequency identified transition states. Thermochemical parameters were derived from these frequency calculations, with only Gibbs free energies (ΔG, 298.15 K) reported.

Single-point energy refinements

Single-point electronic energies were computed at the wB97X-D4 level of theory[31,32], with the def2-QZVPP basis set[33]. The RIJCOSX approximation was used[34], with the def2/J auxiliary basis sets[35]. TightSCF convergence and DefGrid3 integration grids were applied. The CPCM solvation model with THF was explicitly employed for all single-point refinements.

Decomposition analyses

DLPNO-CCSD(T) LED

Local Energy Decomposition (LED) analyses were performed using DLPNO-CCSD(T) with the CPCM(THF) solvation model[36–42]. The def2-TZVP(−f) basis set was applied for correlation[33], with def2-TZVP/C for RI fitting[43]. The def2/J auxiliary basis was used consistently[35]. NormalPNO settings were adopted, with VeryTightSCF convergence. LED decompositions provided electrostatic, exchange, dispersion, induction, and correlation contributions to the interaction energy. Representative DID plots generated from these analyses are included in the SI[44,45].

EDA-NOCV

Energy Decomposition Analyses with Natural Orbitals for Chemical Valence (EDA-NOCV)[46] were carried out at the wB97X-D4/def2-TZVP level using the CPCM(THF) solvation model[31,33]. Systems were partitioned into chemically meaningful fragments with defined charge and spin multiplicities. Decomposition into ΔE_{elstat}, ΔE_{orb}, ΔE_{Pauli}, and ΔE_{disp} was obtained, and NOCV deformation densities were analysed. Dispersion Interaction Density (DID) plots illustrating σ-donation and back-donation pathways are included.

Additional Analyses

QTAIM

Quantum Theory of Atoms in Molecules (QTAIM) analyses were performed with Multiwfn 3.8dev and AIMAll using the r2SCAN-3c wavefunctions[47–49]. The CPCM(THF) solvation model was employed consistently. Bond critical points, electron density ρ(r), Laplacian $\nabla^2\rho$, and associated energy density descriptors were extracted.

NBO

Natural Bond Orbital (NBO) analyses were carried out with NBO 7 interfaced to ORCA on the r2SCAN-3c wavefunctions[50,51]. The CPCM(THF) solvation model was employed consistently. Natural charges, Wiberg bond indices, and second-order donor→acceptor stabilization energies were evaluated.

XYZ coordinates of optimized structures

Complexes are labeled as XCaY, with equatorial ligands (Y) denoted to the right and axial ligands to the left (X) of Ca (corresponding to $[^{Ar*}NONCa]^{2-}$ and including the appropriate counterions, unless denoted with "_anion"). For transition states (denoted with "TS_"), an underscore denotes the breaking bond and in the case of nucleophilic attack, the attacking species is denoted on the right separated by "_A_" denoting attack and "_r" denotes a rearrangement in which the species proceeding it migrates to the other position (e.g. CaTHFr denotes an equatorial to axial THF migration).

BrBiphenyl
Final Single point energy: -3076.042548592849

C	0.38927900	0.19042000	0.01649000
C	1.74431300	0.21802700	-0.34513800
C	2.46127900	1.40558200	-0.32761900
C	1.84735900	2.60298500	0.05337100
C	0.49624400	2.58190000	0.41271000
C	-0.22123400	1.39455800	0.39675700
H	2.24825200	-0.70536600	-0.61637700
H	3.51335400	1.40554300	-0.60283800
H	0.00252000	3.50724600	0.69998200
H	-1.27450500	1.40386800	0.66251700
C	-0.37416800	-1.07474500	0.00248100
C	-0.15119200	-2.03675800	-0.99299200
C	-1.33862500	-1.34071500	0.98505300
C	-0.87177100	-3.22621600	-1.00515800
H	0.57397300	-1.84098700	-1.77834700
C	-2.05617000	-2.53191300	0.97232800
H	-1.51041500	-0.61985700	1.77984800
C	-1.82669500	-3.47965600	-0.02272700
H	-0.69182700	-3.95485600	-1.79083800
H	-2.79237500	-2.72390300	1.74804100
H	-2.38823400	-4.40955400	-0.03277500
C	2.61548900	3.86927300	0.08073600
H	3.68376100	3.72375100	0.23266800
H	2.21267200	4.60479600	0.77498000
Br	2.52062800	4.81428000	-1.71359700

BrCa_anion
Final Single point energy: -6876.878446717740

Ca	10.76926000	15.63420900	6.09477700
O	11.35758500	17.25873700	4.52437900
Br	9.27202800	16.30179100	8.32481800
N	13.05209400	16.09672500	6.24117700
N	9.51145500	15.36103400	4.15080100
C	13.92477200	15.66217000	7.25947800
C	14.94456900	17.30349600	5.17832300
H	15.64202600	16.81814700	5.85106000
C	12.70837100	17.61102400	4.41106700
C	10.60854400	17.33295600	3.34212400
C	8.75371000	14.22440000	3.81417500
C	13.57692500	16.97363900	5.31944600
C	15.39986500	18.19759500	4.21015900
C	14.13358000	16.45061200	8.41892300
C	14.47121200	18.82600300	3.36686000
H	14.81172400	19.53531500	2.62237500
C	10.88714800	18.30429200	2.39861700
C	7.45372900	14.03313000	4.33526600
C	13.99950900	18.96539300	8.02409100
C	13.10360500	18.54779800	3.47388100
C	15.35444300	19.24067800	8.21892600
H	15.97578500	18.52542600	8.75227600
C	9.63621000	16.32701200	3.18099000
C	8.85729100	16.41843900	2.00409800
H	8.08690600	15.66960400	1.86070900
C	9.06473700	17.41192000	1.04904700
C	12.95671800	17.93365400	10.08575400
C	13.22158600	19.88996300	7.32551300
H	12.16609900	19.68095800	7.16176400
C	6.72463900	12.89511600	3.99235200
H	5.72569400	12.76453800	4.40494800
C	6.27163200	16.25906500	4.50162900
C	4.55661800	14.80478300	6.36173800
H	4.12978800	15.51609800	5.66091200
C	13.34109100	17.73474200	8.62022800
H	12.39806100	17.59681200	8.07103600
C	14.55795400	14.39998700	7.19580900
C	15.12987800	21.34037700	7.04756500
H	15.56885400	22.25899000	6.66763500
C	14.21165200	12.01284300	6.50609200
C	15.21522800	13.65607500	4.85297000
C	5.91218000	14.48624800	6.28802400
C	7.24688200	11.91121500	3.15305100
C	14.27825500	13.46066000	6.03271100
H	13.27580400	13.71460800	5.65852400
C	13.78047100	21.06799100	6.83631800
H	13.16055700	21.77360600	6.28974300
C	15.71968900	14.82013100	9.29787400
C	6.86389400	15.08678700	5.26194200
H	7.70355100	15.49814200	5.83799100
C	15.91562600	20.42043200	7.73932600
H	16.97217500	20.61934100	7.89993700
C	15.03085500	16.02759600	9.39872100
H	15.17039900	16.64391200	10.28509400
C	10.09679200	18.34195700	1.24445600
H	10.27915800	19.10916400	0.50159100
C	6.43393800	13.57592300	7.21669500
H	7.49196100	13.32504400	7.17383700
C	15.43882500	14.00552800	8.20418100
H	15.90993600	13.02636100	8.13742800
C	10.76462500	13.29276100	2.57092500
H	11.24663400	13.99044000	3.27274300

C	9.31372600	13.19664800	3.01650900
C	12.01216700	19.29040500	2.70127300
C	8.55576300	12.06950100	2.70010500
H	9.01233000	11.27611000	2.10999500
C	13.28120200	19.07796900	10.81445300
H	13.84268200	19.87852900	10.34231100
C	12.22315000	16.92509300	10.72444600
H	11.95443600	16.03168500	10.16662400
C	16.89573500	18.48389400	4.01667000
C	15.12850400	11.03888800	6.11530300
H	15.92495600	11.29567100	5.42257500
C	17.76245200	17.83769500	5.10516700
H	17.67763800	16.74599100	5.09543200
H	17.48681100	18.19776000	6.10319200
H	18.81371900	18.09315100	4.93007700
C	16.57226100	13.94095700	5.01310900
H	16.97780600	14.08382200	6.01136100
C	14.71363500	13.49683900	3.55953200
H	13.65919100	13.26982700	3.42369700
C	10.97727900	13.88651200	1.19032400
C	8.16439500	17.54549900	-0.18741800
C	12.89240300	19.20890900	12.14925900
H	13.15917700	20.10817900	12.69840200
C	11.48532800	11.95546800	2.73227600
C	6.56138000	17.56203900	4.91029400
H	7.23824500	17.71827300	5.74805600
C	5.41400500	16.07103400	3.41548900
H	5.19197800	15.06154800	3.07688800
C	10.18555200	13.52810200	0.09828800
H	9.33133400	12.87234900	0.24543500
C	3.73896600	14.22128400	7.33152600
H	2.68474700	14.48287900	7.37086800
C	12.16767700	18.19993800	12.77309300
H	11.86306600	18.30278200	13.81106000
C	13.18807000	11.65100800	7.39049000
H	12.46862900	12.40477600	7.70618800
C	16.71789900	14.40360800	10.34473100
H	16.44699700	14.79616800	11.32987900
H	17.71916400	14.78446000	10.10571900
H	16.79026400	13.31378700	10.41250600
C	11.83048600	17.05456500	12.05018600
H	11.25654700	16.26110200	12.52175100
C	4.26664600	13.31538400	8.24456100
H	3.63067200	12.86411300	9.00120900
C	12.13967400	11.30843300	1.68383800
H	12.13185100	11.74578300	0.68999800
C	17.40866400	14.05231800	3.90465000
H	18.46294900	14.27547300	4.04691100
C	15.03113400	9.73410600	6.60132900
H	15.75595300	8.98869700	6.28450900
C	5.62422500	12.99623500	8.18461500
H	6.05194500	12.29664000	8.89793500
C	4.84276700	17.16125500	2.76515500
H	4.17357000	16.99826400	1.92422000
C	5.13547600	18.45833100	3.18197900
H	4.69679000	19.30979300	2.66876900
C	11.44885200	20.39830800	3.62671300
H	12.24243100	21.10773200	3.88808200
H	11.04955100	19.96928500	4.55135500
H	10.64238500	20.93835800	3.11717600
C	7.19467900	16.36582900	-0.33507300
H	6.50326700	16.30281100	0.51180500
H	7.73340300	15.41444000	-0.41448900
H	6.59970600	16.49745400	-1.24580400
C	11.52844700	11.37216200	4.00482300
H	11.02862900	11.86868800	4.83476100
C	15.54304300	13.61756700	2.44852500
H	15.12687100	13.49846200	1.45100700
C	6.00332400	18.65594200	4.25350100
H	6.24745800	19.66374300	4.57897300
C	16.89843400	13.89200000	2.61834700
H	17.55079200	13.98906800	1.75473800
C	12.55466500	19.94935400	1.43139700
H	11.76483200	20.50669900	0.92028800
H	12.96591000	19.20839700	0.73741700
H	13.33948500	20.66850400	1.68209200
C	7.33670200	18.83953400	-0.05662500
H	6.67332400	18.95618900	-0.92295900
H	7.98619300	19.71967600	-0.00140500
H	6.72152700	18.81127500	0.84957000
C	17.33356700	17.91944400	2.65076200
H	18.40576500	18.09166600	2.49314100
H	16.78526400	18.39712600	1.83191200
H	17.14560700	16.84063400	2.60325000
C	17.16171600	20.00045600	4.04164400
H	16.84442800	20.42884400	4.99806800
H	16.63002700	20.52271200	3.24044900
H	18.23374900	20.19408400	3.91346300
C	14.01279600	9.38559800	7.48163300
H	13.93553300	8.36905600	7.85755800
C	6.42850900	10.71019100	2.76066600
H	5.87125000	10.89910100	1.83410800
H	5.69766000	10.45775200	3.53511700
H	7.06498700	9.83713200	2.58561800
C	12.05953900	14.74438800	0.98045700
H	12.67606800	15.04378200	1.82614100
C	12.81646600	10.10666400	1.89959500
H	13.32129800	9.62023300	1.06895500
C	9.01139500	17.62442400	-1.47056800
H	9.60736400	16.71465100	-1.59458400
H	9.69398600	18.47967800	-1.45931800
H	8.35577400	17.73061100	-2.34353100
C	13.08575400	10.35310700	7.87387200
H	12.28085600	10.09210100	8.55603800
C	12.20327100	10.17894300	4.22336300
H	12.24355600	9.75863600	5.22421100
C	12.85153200	9.53756600	3.16752600
H	13.38569300	8.60679500	3.33863900
C	10.48136200	14.00003700	-1.17787700
H	9.85427200	13.71162300	-2.01765800
C	12.35545300	15.22332900	-0.29252300
H	13.19916500	15.89394900	-0.43407100
C	11.57190700	14.84342300	-1.37986400
H	11.80041300	15.21403300	-2.37552600

BrCaF

Final Single point energy: -6976.901512372897

Ca	11.04464500	15.74927900	6.30803000

O	11.57346200	17.31246900	4.53359500
F	10.89827100	13.83018400	7.18952200
N	13.39065700	16.28307600	6.20508100
N	9.69048900	15.44248400	4.36769400
C	14.30932700	15.93750300	7.20737200
C	15.17849600	17.51803900	5.01262800
H	15.92414900	17.07669600	5.66365100
C	12.89308900	17.71422400	4.34440600
C	10.74464300	17.36096000	3.41331700
C	8.90263800	14.30249500	4.17646500
C	13.83043000	17.14459400	5.23683000
C	15.55517500	18.39350700	3.99500400
C	14.55983600	16.81107300	8.29636000
C	14.56465500	18.96319100	3.18135000
H	14.84305000	19.66225200	2.40210000
C	10.94678300	18.30394800	2.42325400
C	7.62278800	14.18735600	4.76220200
C	14.39544900	19.31901500	7.81328700
C	13.21424400	18.63586300	3.36375300
C	15.75622000	19.59761100	7.95351900
H	16.39957300	18.88641700	8.46526900
C	9.75348100	16.35511800	3.35624000
C	8.90492700	16.39933600	2.22295800
H	8.13031700	15.64322400	2.15962300
C	9.05506400	17.35107700	1.21599600
C	13.34262800	18.32723100	9.88742200
C	13.59008300	20.23859000	7.13757500
H	12.52943200	20.02632900	7.01689300
C	6.87900800	13.01803300	4.59927800
H	5.90167000	12.94455600	5.07465000
C	6.29243600	16.34511500	4.73878000
C	4.97043100	15.05888500	7.01310800
H	4.38114600	15.57404600	6.25953200
C	13.75281900	18.09345600	8.43559900
H	12.82130500	17.92144600	7.87667700
C	14.94189200	14.67201200	7.22186600
C	15.48559200	21.68605000	6.77053200
H	15.90937600	22.59985900	6.36255400
C	14.64357600	12.23385300	6.69785400
C	15.43312900	13.81574300	4.88126600
C	6.33837700	14.87514700	6.81441500
C	7.36204300	11.93621100	3.86445800
C	14.60562900	13.65265500	6.14455300
H	13.56397800	13.84927900	5.85402200
C	14.12884700	21.41077200	6.61430800
H	13.48777600	22.10957100	6.08321400
C	16.18121200	15.25430500	9.24080500
C	7.08059000	15.35143100	5.57441200
H	7.95838300	15.90341800	5.93711700
C	16.29757100	20.77320200	7.44050300
H	17.35991300	20.97306800	7.55637300
C	15.48921200	16.46339300	9.27633300
H	15.65126700	17.14245200	10.11224900
C	10.08708100	18.29643700	1.31639000
H	10.21368100	19.04091100	0.53955200
C	7.07763300	14.21801300	7.80749000
H	8.14760900	14.07186200	7.66478700
C	15.86390300	14.35886200	8.22122800
H	16.33824100	13.37889100	8.21003400
C	10.86528500	13.22149700	3.00407300
H	11.37167300	13.93962500	3.66683800
C	9.42678700	13.17691300	3.49365300
C	12.06244400	19.32495900	2.63186100
C	8.65199800	12.02880900	3.33996300
H	9.07963900	11.16742400	2.82839000
C	13.70993400	19.45701700	10.61813200
H	14.31805100	20.22699500	10.15224200
C	12.54927800	17.35789700	10.51560700
H	12.25026300	16.47410500	9.95631400
C	17.02954000	18.71698600	3.71314700
C	15.59471100	11.28961800	6.31465100
H	16.33729400	11.54736600	5.56437500
C	17.97064700	18.14390800	4.78087800
H	17.92218100	17.05056600	4.81845300
H	17.73064700	18.53425700	5.77666100
H	19.00316500	18.42543100	4.54403500
C	16.77341800	14.20377800	4.91022400
H	17.24021900	14.44708600	5.86151700
C	14.84805700	13.52490700	3.64670300
H	13.80668900	13.21329500	3.61560200
C	11.03446200	13.76847900	1.59910300
C	8.08799300	17.42540700	0.02570100
C	13.30445600	19.61191100	11.94544200
H	13.60489000	20.49914400	12.49701700
C	11.57261500	11.88537000	3.19958200
C	6.47077700	17.71266000	4.96440300
H	7.19435400	18.03528800	5.71096100
C	5.37661600	15.94103600	3.76526000
H	5.24001300	14.88152100	3.56396300
C	10.20940900	13.36931000	0.54634400
H	9.37552300	12.69959900	0.74334300
C	4.35035300	14.58997600	8.17289600
H	3.28259900	14.74173200	8.30915000
C	12.51924400	18.64218000	12.55866600
H	12.20011700	18.76448700	13.59020600
C	13.68592300	11.87291400	7.65442500
H	12.92123600	12.59625700	7.93238300
C	17.21844600	14.91895400	10.27971800
H	16.99234900	15.40234400	11.23557900
H	18.21438900	15.26056100	9.96892000
H	17.28108800	13.83860000	10.44427200
C	12.13911900	17.51166700	11.83329000
H	11.51752000	16.74972300	12.29625300
C	5.09196800	13.93708300	9.15159200
H	4.61008700	13.57646400	10.05637500
C	12.07659100	11.12229000	2.14594200
H	11.95817500	11.46936600	1.12361700
C	17.51246200	14.29253800	3.73237800
H	18.55472400	14.59900900	3.77223700
C	15.59966100	10.01388000	6.88159800
H	16.34831800	9.29036600	6.56883800
C	6.46348100	13.75524700	8.96422800
H	7.05615200	13.25407700	9.72517800
C	4.64446900	16.88141900	3.04438700
H	3.93555800	16.54928500	2.29010900
C	4.82733600	18.24257400	3.27774900
H	4.26422500	18.97640600	2.70719000
C	11.51994400	20.44299100	3.55813400

H	12.30600100	21.18050200	3.75971800
H	11.18521700	20.02416600	4.51285400
H	10.67045600	20.94744000	3.08257200
C	7.13511800	16.22444500	-0.03024100
H	6.48736500	16.17844400	0.85178900
H	7.68821900	15.28061800	-0.10246700
H	6.49166200	16.31094100	-0.91346600
C	11.75690100	11.42412300	4.50998700
H	11.38860600	12.02360400	5.34253000
C	15.57857900	13.62290000	2.46624400
H	15.09696000	13.40419600	1.51605600
C	5.74875600	18.65563800	4.23803700
H	5.91018700	19.71523000	4.41891600
C	16.91802000	14.00575200	2.50546200
H	17.49213100	14.08731300	1.58632900
C	12.51272400	19.96066700	1.31482600
H	11.67929200	20.48312100	0.83670300
H	12.89973200	19.20921100	0.61796200
H	13.29297400	20.70592100	1.49446500
C	7.24286000	18.70841400	0.15302300
H	6.52851600	18.78026900	-0.67727400
H	7.87738400	19.60101800	0.13883200
H	6.68080300	18.70434000	1.09394600
C	17.41836000	18.10877600	2.35098400
H	18.47509500	18.30736400	2.13005000
H	16.81327800	18.53264100	1.54246400
H	17.26426300	17.02357600	2.35830900
C	17.24894500	20.24072200	3.66181500
H	16.96535800	20.69992200	4.61464900
H	16.65997800	20.71112500	2.86849700
H	18.30638300	20.46199000	3.47037600
C	14.65288800	9.66757600	7.83966800
H	14.65568100	8.67416200	8.28040500
C	6.52626500	10.70084900	3.65565100
H	7.15227700	9.80537800	3.58652700
H	5.94801700	10.76713600	2.72482400
H	5.81277100	10.56176800	4.47396100
C	12.08557300	14.64789000	1.33037100
H	12.72292500	14.98287200	2.14611300
C	12.74347400	9.92083900	2.39191900
H	13.13114300	9.34216300	1.55725000
C	8.86651900	17.46936800	-1.30224800
H	9.48219800	16.57077600	-1.41556300
H	9.52374000	18.34226200	-1.36247500
H	8.16610300	17.51804600	-2.14529100
C	13.69128500	10.60517100	8.22216900
H	12.93604500	10.34118700	8.95828900
C	12.42401200	10.23102600	4.75572500
H	12.57991500	9.90408900	5.77988100
C	12.91933200	9.47048500	3.69575000
H	13.44733100	8.54054800	3.89006000
C	10.44199600	13.82262300	-0.74961800
H	9.78914100	13.50315700	-1.55806700
C	12.31804900	15.10928500	0.03788100
H	13.13605900	15.80068200	-0.14864100
C	11.50053800	14.69090500	-1.00992500
H	11.67850900	15.04988900	-2.02013500
Br	9.60581500	17.71812300	7.83591700

BrCaTHF_anion

Final Single point energy: -7109.303635859707

Ca	4.98836000	9.04279500	12.86419000
Br	5.86866200	7.44288700	10.68564000
O	4.82940400	7.84430800	14.88093200
O	4.83589800	10.96181500	11.50581100
N	6.91131200	9.37398500	14.23571200
N	2.74007900	8.32686800	13.28172000
C	7.98368300	10.26111000	13.99697900
C	8.08195900	8.67380800	16.29741400
H	8.92938000	9.29367300	16.03008200
C	0.68076400	9.55911000	12.72597600
C	6.98553300	8.65584000	15.40248000
C	1.57824500	8.49117000	12.49138900
C	8.04862300	11.51399100	14.65543500
C	-0.54035900	9.60700400	12.05254900
H	-1.22470800	10.42757000	12.25875700
C	2.54971400	7.49724800	14.36427600
C	8.11062400	7.90885200	17.46270300
C	0.67666900	10.24936600	15.15014500
C	5.88899000	7.04886500	16.92144900
C	5.89687200	7.82499300	15.77727000
C	1.04360200	10.64476900	13.73052700
H	2.14149500	10.71967500	13.71475700
C	1.32294200	6.87702800	14.70011800
H	0.47487500	7.07338200	14.05683200
C	0.51921600	12.02507000	13.33486500
C	9.11264800	12.37974900	14.41224200
H	9.15239400	13.33030900	14.94083000
C	3.52840200	6.40690400	16.35132500
C	1.26151700	7.57629800	11.45900500
C	9.29770300	7.94553100	18.43639300
C	10.07332000	10.82293600	12.88008500
H	10.86532700	10.54625100	12.18705700
C	10.13760400	12.05575000	13.52342500
C	-0.89759500	8.65079100	11.10435600
C	9.02351000	9.92788100	13.09732900
C	1.17850300	6.03952500	15.80306300
C	0.66268300	12.46253000	12.01177300
H	1.06368100	11.78029100	11.26913300
C	-0.65386000	10.03415900	15.51948700
H	-1.43999000	10.12267900	14.77287800
C	0.03830600	7.66664300	10.79473900
H	-0.18134400	6.95797200	9.99811900
C	1.66965300	10.11081700	16.11829600
H	2.70953200	10.23874500	15.83029900
C	-0.16413800	5.38566200	16.16089800
C	3.63152600	7.22375800	15.23955800
C	2.28913400	5.80687200	16.61807000
H	2.19807800	5.14953700	17.47551200
C	2.33318300	6.31000600	9.55064400
C	7.01308300	7.09835600	17.75982800
H	7.02577400	6.48509700	18.65396200
C	6.94731500	11.90365600	15.63099300
H	6.56755700	10.97401400	16.06711500
C	9.47532600	7.46453300	13.35092600
C	-0.02142600	12.91830500	14.26189500
H	-0.14384600	12.61273100	15.29666600
C	5.76070000	12.57787200	14.96540500

C	9.01276500	8.56708600	12.41590700
H	7.96332000	8.34212600	12.18441700
C	2.26468500	6.50565000	11.06180600
H	3.25022800	6.89460400	11.34876200
C	0.28619200	13.74446600	11.62969300
H	0.41095200	14.05560100	10.59561500
C	2.10087000	5.20401300	11.82500700
C	-0.40162800	14.20617300	13.88340300
H	-0.81758400	14.88079400	14.62723000
C	4.72589100	6.12027200	17.25009700
C	-0.98351900	9.71998200	16.83370000
H	-2.02365400	9.55937100	17.10566600
C	10.70449100	7.53994300	14.00989400
H	11.32358100	8.42574700	13.88394300
C	5.88195900	13.39340200	13.84071300
H	6.85378200	13.51181800	13.36868900
C	1.34633000	9.79373100	17.43550300
H	2.13617200	9.68832300	18.17484400
C	7.47449500	12.72836900	16.79855000
C	-1.26381900	5.71386800	15.14298200
H	-1.45918700	6.79148400	15.09487000
H	-2.19431400	5.21634700	15.43936100
H	-0.99929500	5.36607900	14.13768200
C	2.39099800	5.05261200	8.94834800
H	2.33318700	4.15787200	9.56082100
C	9.85970900	6.52398800	18.63231200
H	9.10310100	5.84367300	19.03548500
H	10.70344400	6.54538600	19.33316400
H	10.21155300	6.11533500	17.67935200
C	0.01620200	9.60600900	17.79967000
H	-0.24089600	9.35784000	18.82595100
C	11.14253300	6.49372300	14.81603400
H	12.10355500	6.56412900	15.31928300
C	-0.62744500	5.88519600	17.54310000
H	0.09863800	5.63264600	18.32296900
H	-1.58699200	5.42379800	17.80850700
H	-0.75440900	6.97235400	17.53564600
C	-0.24921400	14.62748900	12.56677400
H	-0.54482200	15.63055000	12.27168100
C	4.50146400	12.43347800	15.55552300
H	4.40188300	11.80652800	16.43979800
C	10.44136300	8.84042200	17.94190900
H	10.83078100	8.49832300	16.97663000
H	11.26226900	8.81127500	18.66725700
H	10.12860600	9.88504500	17.83482300
C	-2.24133100	8.68976100	10.42625000
H	-2.97537400	8.08630500	10.97556300
H	-2.18513700	8.28788500	9.40969200
H	-2.63130100	9.71105300	10.37471200
C	0.89778100	4.49417100	11.82109000
H	0.03660200	4.89740600	11.29354200
C	11.26278100	13.01909700	13.25357700
H	10.99408100	13.72620500	12.45824700
H	12.16654100	12.49302800	12.93104300
H	11.50300900	13.60792700	14.14457600
C	4.76883100	14.05278500	13.31904300
H	4.88053700	14.68478400	12.44141900
C	8.82070600	8.47998000	19.80176000
H	8.40280700	9.48842700	19.70364100
H	9.66119700	8.52376200	20.50552300
H	8.04794400	7.83560600	20.23320600
C	2.42660000	7.44072500	8.72780000
H	2.38501300	8.42782700	9.18139100
C	9.73450300	8.54932200	11.07329300
C	3.39050500	13.08635400	15.03677000
H	2.41873600	12.95313200	15.50280200
C	3.51925500	13.90101600	13.91244700
H	2.64671800	14.40223500	13.50166200
C	10.69651300	7.59580300	10.73665200
H	10.99105800	6.84663100	11.46503700
C	-0.00566000	3.85467600	16.21969700
H	0.31701300	3.46216100	15.25044000
H	-0.96308500	3.38782200	16.48290900
H	0.73266900	3.55547600	16.97065200
C	8.68382800	6.32992300	13.53131800
H	7.72020400	6.27236400	13.02919400
C	11.28583900	7.58742900	9.47090900
H	12.03378200	6.83494700	9.23465200
C	0.79327900	3.27054700	12.47504800
H	-0.14932600	2.72907500	12.45985100
C	7.43454100	14.12387700	16.82417400
H	6.98105600	14.66547000	15.99783700
C	10.34746800	5.36103500	14.98643100
H	10.68638100	4.54538700	15.61953300
C	4.43977500	10.95651900	9.16130100
H	4.26582400	9.95461100	8.76062800
H	4.04126800	11.68562700	8.45091000
C	2.56742100	7.32030600	7.35161200
H	2.64201700	8.21414700	6.73731200
C	3.19067500	4.67042300	12.51466700
H	4.12767400	5.22344500	12.53328500
C	5.99419600	11.59340600	10.90656500
H	6.87767300	11.25656000	11.45870900
H	5.89371100	12.68060000	11.02145800
C	8.04120200	12.05616400	17.88535000
H	8.05853200	10.96875000	17.87244000
C	2.52800400	4.92704800	7.56460000
H	2.56902900	3.93639000	7.11917000
C	2.61585200	6.05723500	6.75966800
H	2.72406400	5.95901700	5.68294600
C	1.89024000	2.74144300	13.15385200
H	1.80687700	1.78816800	13.66896500
C	3.08838600	3.45031900	13.17881300
H	3.94654300	3.05358500	13.71541000
C	9.11205500	5.28568200	14.34783600
H	8.48026600	4.41157800	14.48348300
C	5.94863200	11.16990800	9.44100200
H	6.39532300	11.93018000	8.79456500
H	6.48843400	10.22961200	9.30336600
C	7.96663200	14.82931500	17.90271000
H	7.92827600	15.91554500	17.90535800
C	5.18129600	4.65967000	17.02227100
H	6.03824700	4.42014000	17.66178200
H	5.47646400	4.51317400	15.97739100
H	4.36627100	3.96442100	17.25204300
C	8.57255600	12.75593200	18.96342900
H	9.00738600	12.21204400	19.79838600
C	8.54006200	14.14997000	18.97459000

H	8.95062000	14.70125600	19.81609000
C	10.91881700	8.52889700	8.51618200
H	11.37605200	8.52077800	7.53055100
C	4.31757600	6.29898000	18.72821200
H	3.50434500	5.61928000	18.99578600
H	3.98350700	7.32626600	18.90959400
H	5.15497200	6.08368900	19.39702400
C	3.77311300	11.12110700	10.53354100
H	3.34542800	12.12507200	10.65887100
H	3.00592400	10.37084900	10.75637600
C	9.37189800	9.48921100	10.09905800
H	8.62710900	10.24106200	10.34312300
C	9.95217700	9.48275200	8.83753900
H	9.64859300	10.22241100	8.10105200

Br_anion

Final Single point energy: -2574.312714622228

Br	16.07104000	0.83903000	12.51927000

Brpentane

Final Single point energy: -2771.240558773510

C	-1.97710500	-2.05744500	-0.00771900
H	-1.63474600	-3.09807700	-0.04061900
H	-1.63384800	-1.56469200	-0.92457600
H	-3.07192900	-2.06384300	-0.02002000
C	-1.43853000	-1.34399500	1.23048800
H	-1.81298500	-0.31188500	1.25673900
H	-1.81804800	-1.83491300	2.13672000
C	0.09003400	-1.32417900	1.27336400
H	0.47317500	-0.83161200	0.36860000
H	0.46822500	-2.35587700	1.25328300
C	0.62764700	-0.60454200	2.51627800
H	0.25668900	-1.10085400	3.42110000
H	0.25854700	0.42790300	2.53492300
C	2.13897400	-0.60920900	2.51089600
H	2.56005100	-0.06626000	1.66381500
H	2.55862500	-1.61480000	2.55909000
Br	2.87651400	0.31967300	4.11950500

CaBr_anion

Final Single point energy: -6876.877968153426

Ca	11.03924500	15.27818400	5.86133200
O	11.67232400	16.84232200	4.20048000
Br	10.56269800	13.29254400	7.74522200
N	13.21322500	16.02355800	6.14698200
N	9.58187700	15.28089600	4.06242800
C	14.01643100	15.60411900	7.22386000
C	15.04430800	17.50085900	5.36811400
H	15.68220900	17.15478700	6.17294100
C	12.93760600	17.42117900	4.22731800
C	10.87610400	17.03053900	3.07519400
C	8.70980800	14.19728900	3.86396400
C	13.74314800	16.96202600	5.29639700
C	15.51125300	18.43019700	4.43781100
C	14.09444700	16.35520600	8.41828900
C	14.65807700	18.84782500	3.41167300
H	15.00506600	19.57876400	2.68942000
C	11.17940200	17.94994200	2.09014000
C	7.47448000	14.12595300	4.55050900
C	14.01383400	18.91770200	8.33959500
C	13.35618600	18.33942800	3.28463000
C	15.31382000	19.13051400	8.80027100
H	15.85409000	18.32180500	9.28409800
C	9.75423200	16.17083900	3.03054400
C	8.89821300	16.31809300	1.92144100
H	8.03157900	15.66848100	1.87461300
C	9.13703700	17.26770200	0.92682900
C	12.51011700	17.61071200	9.90305100
C	13.35196400	19.96962900	7.69981800
H	12.34243800	19.81138100	7.32539400
C	6.65345300	13.01102100	4.39549400
H	5.70542900	12.97555300	4.92914100
C	6.53097200	16.46936900	4.63812100
C	4.76631500	15.23027700	6.61009100
H	4.34577200	15.86112500	5.83256400
C	13.26196100	17.61824300	8.57343300
H	12.50015200	17.56899600	7.78320700
C	14.69013200	14.36003500	7.16769800
C	15.25679900	21.41515100	8.01512900
H	15.74000100	22.38011000	7.88792600
C	14.72942500	11.99375900	6.22437400
C	15.28413300	13.98406300	4.74351800
C	6.11157000	14.86539800	6.55827300
C	7.02093200	11.93157200	3.59125800
C	14.50381300	13.47493600	5.94015200
H	13.44199900	13.56003200	5.66165000
C	13.96531800	21.20737900	7.53460600
H	13.43607900	22.00985400	7.02744300
C	15.62469100	14.72641700	9.38889000
C	7.05484400	15.29076200	5.43837800
H	7.96860800	15.64789100	5.93321900
C	15.92964400	20.37020600	8.64258700
H	16.94302600	20.51721900	9.00734700
C	14.88289400	15.90106800	9.47719100
H	14.89903300	16.47006300	10.40560600
C	10.27930200	18.06916500	1.01970100
H	10.47543300	18.81336200	0.25539100
C	6.62644600	14.06282400	7.58397400
H	7.67609100	13.77489500	7.55711200
C	15.49750400	13.95945400	8.22934200
H	16.01909500	13.00674700	8.16680800
C	10.46712800	13.08327100	2.40230000
H	11.05852200	13.85547100	2.91490800
C	9.10123300	13.09096500	3.07031600
C	12.43589500	18.81334900	2.16212500
C	8.25854800	11.98526400	2.95370800
H	8.59235300	11.12924500	2.36854200
C	12.69207500	18.57628700	10.89292200
H	13.39589200	19.38807600	10.73313100
C	11.59170000	16.57947100	10.13831000
H	11.44638600	15.80658000	9.38471500
C	16.93658700	18.99682900	4.49549700
C	15.60603900	11.20275100	5.48252000
H	16.18688900	11.64746600	4.68019900
C	17.74922100	18.42116200	5.66170100
H	17.85175100	17.33284000	5.58167700
H	17.28946200	18.65595900	6.62801600
H	18.75507900	18.85613100	5.65221100

C	16.64311300	14.28669600	4.84905000
H	17.13902400	14.18745300	5.81225400
C	14.65699300	14.13086100	3.50628900
H	13.59612000	13.90216000	3.41326100
C	10.47010000	13.47294500	0.93370900
C	8.16633000	17.48361500	-0.24230600
C	11.97773600	18.51125900	12.09078800
H	12.13719900	19.27167600	12.85090700
C	11.19763300	11.76353200	2.64300800
C	6.93178500	17.76453800	4.97025400
H	7.65604400	17.90901500	5.76972400
C	5.61421400	16.29611600	3.59898600
H	5.30921600	15.29071000	3.31767700
C	9.44314200	13.12629700	0.05579500
H	8.55688600	12.62484400	0.43440200
C	3.95073300	14.79516300	7.65619400
H	2.90478700	15.08989200	7.67771100
C	11.06646600	17.48463900	12.31259800
H	10.50876500	17.43657600	13.24386300
C	13.98187700	11.38518100	7.24150000
H	13.28156700	11.98625100	7.81654700
C	16.52169500	14.28298000	10.51362700
H	16.21467700	14.73004900	11.46393900
H	17.56123000	14.58267600	10.32888900
H	16.51270500	13.19376500	10.62329200
C	10.87420600	16.51626100	11.32598000
H	10.16448800	15.70816400	11.48331500
C	4.47043000	13.99405900	8.66727300
H	3.83577300	13.65855400	9.48295100
C	11.55782200	10.89176200	1.61499100
H	11.31096400	11.13969600	0.58674800
C	17.36335600	14.71461400	3.73811800
H	18.42135900	14.94384900	3.83591800
C	15.74011400	9.83962500	5.75245300
H	16.42670700	9.24160400	5.15886700
C	5.81736500	13.63130500	8.62786100
H	6.23918800	13.01226300	9.41552400
C	5.08835100	17.39559000	2.92597600
H	4.36922000	17.24474200	2.12508200
C	5.49099600	18.68483000	3.26762800
H	5.08755300	19.54266700	2.73651400
C	12.02679800	20.27897800	2.43316200
H	12.91307600	20.92027300	2.49260900
H	11.48174200	20.35298100	3.38039600
H	11.38003600	20.65105900	1.63088300
C	7.06304900	16.41940900	-0.29113600
H	6.43820200	16.44146400	0.60772800
H	7.48321200	15.41264500	-0.39611600
H	6.41516600	16.60937000	-1.15432900
C	11.53532700	11.41861600	3.95727400
H	11.25065800	12.07732300	4.77753000
C	15.36977000	14.57471300	2.39509600
H	14.86443300	14.69570400	1.44045800
C	6.42278600	18.86605000	4.28722200
H	6.75351900	19.86681700	4.55216600
C	16.72764600	14.86404000	2.50681300
H	17.28571800	15.21027700	1.64107600
C	13.18473900	18.73565300	0.81484500
H	12.55113600	19.08473100	-0.00520900
H	13.48489700	17.70302000	0.60558100
H	14.08177300	19.36105600	0.82635600
C	7.50225700	18.86550300	-0.08631000
H	6.79603300	19.04505300	-0.90685200
H	8.24943500	19.66636300	-0.09614000
H	6.95440400	18.92218200	0.86086700
C	17.67886400	18.66116700	3.18699700
H	18.70051100	19.05946500	3.22034800
H	17.17428700	19.09256400	2.31653100
H	17.73468700	17.57672600	3.04381400
C	16.88046300	20.52776900	4.65734200
H	16.35618200	20.79883800	5.57990900
H	16.36111200	21.00163700	3.81804000
H	17.89610400	20.94057600	4.70380700
C	14.99949500	9.24758400	6.76897800
H	15.10326700	8.18637600	6.97856400
C	6.13494700	10.71991900	3.47229600
H	6.31165600	10.18922900	2.53186000
H	5.07701400	10.99655500	3.52109400
H	6.32501700	10.01255500	4.28961500
C	11.59016700	14.13638000	0.42374100
H	12.38974500	14.42230600	1.10413300
C	12.23816900	9.70504800	1.89302000
H	12.50876800	9.03949300	1.07736700
C	8.92454700	17.44076400	-1.58224300
H	9.42951400	16.47706600	-1.70664900
H	9.67810000	18.23145500	-1.64980100
H	8.22260000	17.57502700	-2.41443100
C	14.11564400	10.02987000	7.51414100
H	13.52157100	9.57906200	8.30500700
C	12.21915800	10.24249600	4.23717100
H	12.48833800	10.00678400	5.26279500
C	12.57437000	9.37743700	3.20185600
H	13.11313700	8.45891000	3.41872900
C	9.54126200	13.42083500	-1.30296400
H	8.73075000	13.14452300	-1.97251400
C	11.69032800	14.43687000	-0.93024000
H	12.56636500	14.96007900	-1.30496900
C	10.66655800	14.07027300	-1.80279900
H	10.74014300	14.30253300	-2.86180000

CaF_anion

Final Single point energy: -4402.566619812323

Ca	10.88640600	15.43312000	6.04939600
O	11.39762500	17.19866100	4.50426800
F	10.10585400	14.72381200	7.85351400
N	13.16360300	15.98265300	6.10124600
N	9.54124800	15.31870800	4.13585600
C	13.98855500	15.60716000	7.17192700
C	14.99694300	17.30362900	5.08599200
H	15.71611300	16.80211000	5.72414500
C	12.73481800	17.58528000	4.37260600
C	10.62002600	17.30259600	3.34488700
C	8.77617600	14.18272000	3.83156300
C	13.64130100	16.93041000	5.23097600
C	15.41315900	18.24490900	4.14553700
C	14.16912700	16.46509200	8.28598000
C	14.45239000	18.88177100	3.34519600
H	14.76147800	19.62452900	2.61983200

C	10.86519300	18.30308800	2.42238900
C	7.49593300	13.99539600	4.40205200
C	14.25820800	19.00872600	7.94177100
C	13.09340800	18.56626500	3.46577800
C	15.61505400	19.13207900	8.24209600
H	16.13674300	18.30891100	8.72236500
C	9.64715500	16.29522500	3.18017000
C	8.85012400	16.40209300	2.01666600
H	8.08658400	15.64657900	1.86961400
C	9.03618800	17.41482600	1.07724900
C	12.74434900	17.97523800	9.68710900
C	13.61482600	20.07498600	7.30602600
H	12.55857600	19.98597800	7.05892500
C	6.76788500	12.84057100	4.12060500
H	5.78707100	12.71050100	4.57496500
C	6.27332800	16.20788300	4.56885400
C	4.67280500	14.52479400	6.39732300
H	4.16222400	15.01550700	5.57319300
C	13.43408200	17.79604400	8.33752900
H	12.63274700	17.72078900	7.59009700
C	14.55875200	14.31465300	7.22963300
C	15.65895700	21.35533700	7.29570100
H	16.20332600	22.26090300	7.04189700
C	14.29937000	11.89726400	6.54844400
C	15.24307600	13.59078900	4.90330200
C	6.06727200	14.48777300	6.42539600
C	7.26933800	11.83999700	3.28715400
C	14.31687300	13.34609800	6.08158000
H	13.30621300	13.55584000	5.70263400
C	14.30643300	21.23674600	6.97966500
H	13.79004700	22.04983200	6.47605400
C	15.56764500	14.80375700	9.39444500
C	6.94044500	15.07166900	5.32382200
H	7.80874200	15.51708300	5.82606100
C	16.30978500	20.29764600	7.92488000
H	17.36733600	20.37513900	8.16415100
C	14.94634200	16.05143900	9.36692200
H	15.04230800	16.70976400	10.22934400
C	10.05729700	18.35574500	1.28005100
H	10.21747000	19.14286300	0.55299800
C	6.70181400	13.86521400	7.50750500
H	7.79035800	13.84946600	7.54682800
C	15.33909500	13.94092500	8.32305100
H	15.76699300	12.94027700	8.34712500
C	10.76134200	13.22968900	2.57160800
H	11.25359100	13.93339500	3.26081300
C	9.32065400	13.13494500	3.04861000
C	11.97033700	19.30783300	2.74057000
C	8.56022200	11.99623700	2.78388600
H	9.00253700	11.19140300	2.19835000
C	13.15297600	18.91389300	10.63435600
H	13.98544100	19.57585900	10.41197700
C	11.66266900	17.13940800	9.99332600
H	11.33211100	16.39689300	9.26717500
C	16.89864800	18.56272600	3.92618200
C	15.24596800	10.95526600	6.15058900
H	16.04098800	11.24587600	5.46976000
C	17.79939500	17.91146400	4.98341700
H	17.73649400	16.81863700	4.95148300
H	17.53550300	18.24413600	5.99385300
H	18.84173100	18.19198000	4.79374200
C	16.59325600	13.90115800	5.07402700
H	16.99431100	14.01552100	6.07824900
C	14.74196300	13.47038700	3.60560000
H	13.69088000	13.23090600	3.46204200
C	10.94241100	13.82846800	1.18929700
C	8.11953800	17.56019700	-0.14613000
C	12.50169400	19.01190300	11.86483300
H	12.83597800	19.74752200	12.59182400
C	11.50053300	11.90148300	2.72334700
C	6.47692300	17.52296200	4.99347200
H	7.13791400	17.71279600	5.83701500
C	5.43690400	15.97943000	3.47427100
H	5.28620700	14.96310700	3.11804500
C	10.12607100	13.47336400	0.11478500
H	9.28127800	12.80885200	0.27776900
C	3.92604400	13.94013500	7.42042500
H	2.84046200	13.97745600	7.38129600
C	11.42848700	18.17780300	12.16048700
H	10.91856800	18.25767000	13.11668800
C	13.27714000	11.49423100	7.41683600
H	12.53141000	12.22196400	7.73278700
C	16.44363000	14.39656900	10.54908300
H	16.12646900	14.88292600	11.47696600
H	17.48854300	14.68201400	10.37141200
H	16.42271200	13.31288400	10.70072500
C	11.00886900	17.24033900	11.21552800
H	10.16826100	16.58586900	11.43123200
C	4.56429800	13.31689800	8.48833600
H	3.98225000	12.86567700	9.28731800
C	12.16422800	11.27446900	1.66850300
H	12.13793700	11.71458800	0.67618800
C	17.42557300	14.07397200	3.97032300
H	18.47506100	14.31425100	4.11972200
C	15.17736300	9.63942900	6.61138500
H	15.92340500	8.91834000	6.28764700
C	5.95850300	13.28492400	8.52931600
H	6.46843200	12.81154400	9.36438100
C	4.80313700	17.03970000	2.83126300
H	4.15229400	16.84438000	1.98288900
C	5.01161900	18.34756100	3.26290500
H	4.52642000	19.17581000	2.75368400
C	11.39527100	20.36331400	3.71989600
H	12.17615600	21.08039700	3.99965000
H	11.02164500	19.88573100	4.63130700
H	10.56784300	20.90408900	3.24606400
C	7.16839700	16.36736600	-0.30917300
H	6.48842500	16.27307400	0.54401300
H	7.72299100	15.42789200	-0.41572000
H	6.56046100	16.50845500	-1.20989900
C	11.56666300	11.31401700	3.99349200
H	11.05674200	11.79078600	4.82913600
C	15.56690100	13.65441100	2.49974700
H	15.15215300	13.56609800	1.49847800
C	5.85749100	18.58698100	4.34393900
H	6.03733400	19.60455300	4.68066300
C	16.91596400	13.95361300	2.67929700
H	17.56425800	14.09969400	1.81955700

C	12.47061300	20.03021700	1.48840900
H	11.65548000	20.58308800	1.01321100
H	12.89036000	19.32921100	0.75879400
H	13.23890700	20.76210100	1.75327300
C	7.27084600	18.83632300	0.02229000
H	6.59486300	18.96012500	-0.83328600
H	7.90526300	19.72656000	0.08969600
H	6.66714300	18.77699200	0.93484000
C	17.31566500	18.02840200	2.54138800
H	18.38123300	18.22079300	2.36334900
H	16.74169700	18.50989900	1.74252500
H	17.14413200	16.94734100	2.48032600
C	17.14000600	20.08276200	3.97188500
H	16.83837300	20.49051800	4.94263000
H	16.58225300	20.60948100	3.19165300
H	18.20548600	20.29700500	3.82319500
C	14.15994600	9.24935700	7.47521600
H	14.10464400	8.22418500	7.83109600
C	6.44829200	10.62263300	2.95520400
H	5.84688500	10.78751100	2.05192100
H	5.75642900	10.37679500	3.76683700
H	7.08642000	9.75342600	2.76763300
C	12.01272200	14.69671700	0.96127100
H	12.64874600	14.99028500	1.79460900
C	12.87453700	10.09069600	1.87573500
H	13.38607300	9.62035300	1.03994700
C	8.95015000	17.68112100	-1.43680000
H	9.56022700	16.78459700	-1.58726900
H	9.61794000	18.54772000	-1.41495800
H	8.28299800	17.79402200	-2.30015500
C	13.20543000	10.18585700	7.87698500
H	12.40078900	9.89183600	8.54588700
C	12.27656000	10.13952400	4.20402600
H	12.33449700	9.71695700	5.20320700
C	12.93540600	9.51970700	3.14185000
H	13.49678400	8.60395400	3.30660400
C	10.38469400	13.96184900	-1.16343000
H	9.73918700	13.67647500	-1.99018300
C	12.27082000	15.19260600	-0.31322000
H	13.10434900	15.87264500	-0.46942100
C	11.46141200	14.81825400	-1.38370200
H	11.66030500	15.20213100	-2.38067600

CaFCa

Final Single point energy: -7813.553280175238

Ca	12.53572300	17.53619500	9.91440200
Ca	13.97988100	16.71422100	5.88746700
F	13.15495900	16.91308900	7.90504600
O	13.73592800	14.47478400	5.10096400
O	14.66126700	18.67044700	9.94285600
O	14.62683700	18.90465600	5.23102600
O	10.22775500	17.17670100	10.63180300
N	16.35413800	17.01185100	5.84881200
N	12.38307500	17.77960000	4.49531700
N	12.27692200	15.54455900	11.20208200
N	11.38226700	19.56219300	10.46091700
C	11.04163500	15.21386000	11.68820100
C	9.93569100	16.04057800	11.39119900
C	8.63855100	15.77985400	11.79868100
C	8.40895500	14.65258200	12.59799900
H	7.40029100	14.42656200	12.92259100
C	13.73085300	19.75245100	4.59331800
C	9.46712700	13.81269900	12.97173100
C	13.99331100	21.08757100	4.38675900
C	12.52698700	19.10394300	4.20233900
C	15.92397500	19.34347800	5.44590700
C	13.28540000	14.57170900	11.33762900
C	15.28931100	21.73108100	4.87846300
C	11.58101600	19.91913700	3.55191100
H	10.64912400	19.45573000	3.23908100
C	10.75329900	14.09936100	12.51731400
H	11.58506600	13.46260700	12.79465900
C	17.69385000	15.19175500	6.81106900
C	10.05511400	19.53890500	10.77036300
C	16.29547800	20.66256900	5.30058500
C	11.79698500	21.28478800	3.33379400
C	16.82272700	18.29885600	5.79250500
C	14.40885300	14.83687800	12.16567600
C	18.55703400	20.03292000	5.97977900
C	17.63326500	21.00032100	5.58708000
H	17.93101700	22.03830700	5.51192700
C	7.05553300	21.81286700	11.59897100
C	11.27045100	17.10225800	3.96414700
C	7.88728900	20.53890000	11.39463700
C	9.17523100	12.58116300	13.84126900
C	17.89569800	15.73079600	4.43436900
C	15.42261700	13.88182300	12.27110700
H	16.28441500	14.07476600	12.90265500
C	9.23398300	20.65913300	11.03902200
H	9.69057900	21.64162400	10.96287100
C	12.09115400	13.02746700	9.66158800
H	11.34509200	13.82376700	9.74079400
C	11.84052300	21.69449100	9.31584100
C	14.25747800	12.41868600	10.76813400
H	14.21474400	11.48294500	10.21430500
C	18.79507800	14.67249200	4.29772600
H	19.23060600	14.46540300	3.32266500
C	18.14561200	18.69774800	6.06140800
H	18.85507000	17.92235800	6.33840900
C	15.34936300	12.67276600	11.58771900
H	16.14633600	11.94017400	11.68495800
C	17.09953100	15.45960600	8.17683600
H	16.72640300	16.49032900	8.15238700
C	15.89568800	22.59990900	3.75656200
H	16.12659500	21.98662200	2.87905900
H	16.81618400	23.08541300	4.09198900
H	15.20189300	23.38928700	3.45442600
C	10.86111200	21.35027500	8.21041700
H	10.09534300	20.69284300	8.63301500
C	18.57640300	14.12558000	6.62383500
H	18.84361300	13.49460200	7.46816300
C	9.43287200	22.08359800	3.55008700
H	9.07174600	21.06164200	3.70559300
H	8.62593500	22.66566500	3.08762100
H	9.65301900	22.51794700	4.53159400
C	10.35129800	21.49817000	1.28740900
H	11.23880100	21.47457500	0.64421600
H	9.57870900	22.09606600	0.78874700

H	9.97613800	20.47452300	1.38320500
C	6.25414600	16.59711600	12.11487200
H	5.87000300	15.57321700	12.10546200
H	5.47098700	17.23285900	11.69209500
H	6.41994400	16.89678000	13.15554100
C	19.13410000	13.86445800	5.37804400
H	19.82832200	13.03811500	5.24901500
C	11.24086100	16.73972100	2.59052300
C	10.21515400	16.68189700	4.81075700
C	13.56773700	23.15681300	10.19612800
H	14.16875400	24.05829000	10.10873200
C	11.09385900	23.57129400	2.44660700
H	11.29887900	24.07697200	3.39692300
H	10.27349500	24.10524700	1.95433300
H	11.98194600	23.65725100	1.81028500
C	15.85943300	16.44693200	13.52803200
H	15.85454600	17.44670500	13.97607300
H	16.63461400	16.42192800	12.75491400
H	16.14227400	15.73777400	14.31465300
C	14.83996100	13.54071000	4.89963000
H	14.99238600	12.97016900	5.82628600
H	15.73823500	14.12648500	4.68180200
C	20.00884500	20.38313500	6.33039800
C	12.37523600	17.13255000	1.66030200
H	12.89689500	17.98234100	2.10925000
C	17.52345900	16.54543800	3.20769400
H	16.67634900	17.18333700	3.48487000
C	10.45171000	11.84517300	14.26830000
H	11.00401500	11.44730700	13.41009500
H	10.18533300	11.00024900	14.91313000
H	11.12131900	12.50439800	14.83354100
C	10.14565500	22.57471800	7.63037600
H	9.71906400	23.20311100	8.41998400
H	9.33193500	22.24998300	6.97242100
H	10.82289400	23.19388900	7.03018500
C	7.78039800	22.79421100	12.53905100
H	7.95034200	22.33916100	13.52073500
H	7.17158300	23.69520000	12.68075100
H	8.74988500	23.10596500	12.13939400
C	11.57097600	20.58185400	7.09118400
H	12.32504200	21.21091200	6.60653300
H	10.86074700	20.27088900	6.31833200
H	12.07339600	19.68273500	7.46783800
C	6.85623400	22.49254200	10.22967100
H	7.81820300	22.76781900	9.78621300
H	6.25289900	23.40251200	10.33750200
H	6.34324300	21.81741000	9.53505800
C	12.50136100	13.87161800	4.58241700
H	11.75776500	13.86553100	5.38425700
H	12.14025900	14.50557500	3.76573400
C	11.40121700	11.69936500	9.99961700
H	10.53092000	11.55006700	9.34995400
H	11.05816800	11.68870900	11.03830900
H	12.07719400	10.84905800	9.85151300
C	13.74425100	22.29894800	11.27712200
H	14.48479500	22.54803900	12.03206700
C	12.58655800	13.00959500	8.20847900
H	13.37432100	12.26035000	8.06466700
H	12.99075800	13.98484700	7.92017800
H	11.75921100	12.76894200	7.53028500
C	5.67186300	21.52366600	12.19575900
H	5.06054500	20.90795800	11.52745200
H	5.14005500	22.46864900	12.35317500
H	5.74706800	21.01294700	13.16319700
C	15.89728200	14.54404300	8.42274600
H	16.20921200	13.49314900	8.46264100
H	15.16409000	14.63091700	7.61300300
H	15.39044500	14.78082400	9.36551200
C	18.11702900	15.33481700	9.31487300
H	17.66145800	15.62932100	10.26740500
H	18.98916800	15.97497100	9.13944100
H	18.46843000	14.30385400	9.43367000
C	10.15926600	17.09012200	6.27099600
H	11.05402700	17.68676200	6.47527200
C	15.93292300	18.19937200	10.47677400
H	15.98396800	17.11155100	10.34683500
H	15.94295700	18.42966500	11.54669300
C	14.92206600	19.60863400	8.85902800
H	14.12162800	20.35376700	8.87191700
H	14.91118100	19.06084100	7.90676700
C	14.48397800	20.36904500	13.33882500
H	14.57250200	21.33081300	13.85842700
H	15.32815300	20.27775400	12.64731400
H	14.57279800	19.58008300	14.09467600
C	17.02840700	18.94811600	9.71648500
H	17.86477700	19.20912200	10.37068400
H	17.41545400	18.34653200	8.88791600
C	11.99371700	20.49689900	13.61031100
H	12.05319100	19.80725400	14.46257400
H	11.02031100	20.37379500	13.12592700
H	12.05606300	21.52083800	14.00058900
C	13.38428900	15.98083500	1.54358400
H	13.81334600	15.73510300	2.52198200
H	14.20661400	16.25091100	0.87164100
H	12.89885200	15.07933900	1.14857700
C	18.67862800	17.45553000	2.76436600
H	19.54459300	16.85746200	2.45376900
H	18.98857100	18.11612700	3.57947500
H	18.37384900	18.07596300	1.91292700
C	11.89275000	17.57165500	0.27365400
H	11.46941300	16.73780500	-0.29750400
H	12.73396600	17.97039000	-0.30461600
H	11.12958900	18.35406700	0.35020900
C	14.37711400	12.63996800	3.77137200
H	14.92078900	11.69144800	3.75341000
H	14.50548200	13.14205300	2.80529800
C	20.96556200	19.62471300	5.39048000
H	20.83972000	18.54061900	5.47717600
H	20.78225700	19.90410900	4.34658500
H	22.00731600	19.86675500	5.63441400
C	7.53134000	16.69589100	11.27785000
C	17.32632300	16.00119000	5.70895100
C	12.99683800	21.85825100	3.75274800
H	13.17549600	22.91550500	3.60509300
C	7.31943600	19.26567900	11.49649100
H	6.28134700	19.15202300	11.77682300
C	9.40840500	18.28315600	10.87285400
C	13.22644700	13.34670000	10.62092700

C	10.69115000	22.10729400	2.66090900
C	8.08651600	18.11787200	11.23397600
C	12.03717300	20.80683700	10.40216700
C	7.19114500	16.26276400	9.82988000
H	8.07390800	16.32102500	9.18786000
H	6.41759500	16.91874700	9.41372000
H	6.82273700	15.23025500	9.82243700
C	12.61366900	22.85448900	9.23145400
H	12.47764500	23.52909000	8.39007100
C	10.20243700	15.94095100	2.11401800
H	10.19355000	15.64038600	1.06901300
C	14.47138900	16.12631300	12.96900100
H	14.18291200	16.95163800	12.30013800
C	8.29501200	11.60280700	13.03881300
H	7.33930300	12.06248900	12.76646000
H	8.08622700	10.70288500	13.63047500
H	8.80195800	11.29969800	12.11573300
C	9.18260300	15.50222300	2.95529000
H	8.38339000	14.87574000	2.56769200
C	14.97727600	22.62909000	6.09814200
H	14.23662400	23.39263500	5.83449400
H	15.88723400	23.13069400	6.44679200
H	14.57623600	22.03232800	6.92415400
C	9.19419200	15.88062400	4.29063600
H	8.39005900	15.55133500	4.94564600
C	12.98937600	21.13213500	11.40358300
C	8.42679300	12.99274100	15.12322600
H	9.04816200	13.65561000	15.73509800
H	8.18805000	12.10268600	15.71775700
H	7.48971200	13.51310300	14.90272800
C	13.14028600	20.23886900	12.62071700
H	13.04164800	19.19880100	12.27936000
C	17.07762900	15.65340300	2.04095400
H	16.71435300	16.27104700	1.21189200
H	16.26850000	14.97877200	2.34116800
H	17.90532300	15.04367500	1.66191200
C	13.45256500	16.11763200	14.11712300
H	13.70261000	15.32309000	14.83097300
H	12.43649300	15.94643000	13.75425200
H	13.47121500	17.07727900	14.64935300
C	8.93311400	17.96803500	6.56137000
H	8.90357900	18.83757800	5.89475700
H	8.95762500	18.32975800	7.59768200
H	8.00198000	17.40424200	6.42600600
C	16.29725200	20.17359400	9.15748500
H	16.22175700	20.96765400	9.90930500
H	16.77645500	20.56988200	8.25689100
C	10.18072800	15.87238600	7.20384300
H	9.30150300	15.23535200	7.04828600
H	10.17840600	16.18869700	8.25347700
H	11.07584400	15.26494000	7.04335000
C	20.30104400	21.88280900	6.19696200
H	19.67354500	22.47859100	6.86933600
H	21.34795400	22.07321600	6.45807600
H	20.14052300	22.23468300	5.17182900
C	20.29426200	19.96599200	7.78606800
H	20.15143500	18.88996900	7.92806600
H	21.32824800	20.21174800	8.05758100
H	19.62223800	20.49120900	8.47495900
C	12.89068800	12.47697700	4.10491800
H	12.28829400	12.16300800	3.24823000
H	12.76366100	11.74455900	4.91032300
K	10.51001300	19.16315900	17.95696500
O	8.74428600	18.72732000	15.76765900
O	10.83249400	16.85071300	16.31344300
O	8.61199500	20.14162500	19.88353700
O	10.21526600	17.83593100	20.49009500
O	13.30731100	19.77372800	18.22120400
O	11.49919000	21.71617100	17.13958000
N	8.55509000	21.35067100	17.16643300
N	12.48240000	16.95311000	18.77104300
C	9.27279700	17.82979100	14.78771800
H	10.11436900	18.30229000	14.25573800
H	8.50132200	17.57943800	14.04405400
C	9.72232500	16.56584200	15.45929600
H	8.89423500	16.13436700	16.04677200
H	10.00817400	15.83747400	14.68276300
C	7.59153500	20.78902600	16.20317800
H	7.02124500	21.59091600	15.69297200
H	6.86048500	20.18342900	16.75041100
C	7.84278900	21.83130200	18.36270600
H	6.93604300	22.40487500	18.08664900
H	8.49652500	22.51857500	18.91086800
C	11.29220500	15.67288700	16.97509200
H	11.46939000	14.87293400	16.23606700
H	10.51858800	15.31192300	17.67350200
C	14.16921600	18.64825900	18.03676900
H	15.21482700	18.94621600	18.21844300
H	14.10099900	18.29635600	16.99359800
C	9.55145500	18.62620500	21.47544600
H	10.20730400	19.44585400	21.81404600
H	9.29511200	18.00756000	22.35087200
C	12.59925300	15.97332800	17.67708300
H	13.03347000	15.01957500	18.03591300
H	13.28897700	16.36964100	16.92644700
C	11.97982400	16.28897400	19.98523500
H	12.77263400	15.68792400	20.47283900
H	11.18488500	15.59087800	19.69879000
C	8.28394000	19.18606600	20.89095400
H	7.67302600	18.37384500	20.46254800
H	7.70276700	19.66518700	21.69567300
C	9.29887800	22.46098100	16.54638700
H	8.67578200	23.37477300	16.47993300
H	9.55971400	22.18323900	15.51898700
C	13.71864600	20.88155800	17.42081700
H	13.71272500	20.60569500	16.35344600
H	14.74282100	21.18730400	17.69065600
C	10.58895900	22.81038800	17.25872000
H	11.01779900	23.70664500	16.78126000
H	10.42827400	23.04725600	18.32287300
C	13.79703600	17.56557800	19.02895500
H	14.60074600	16.80358400	19.03193000
H	13.79033100	18.02110500	20.02531300
C	12.78842600	22.04046600	17.65552800
H	12.72401700	22.26798300	18.73295000
H	13.19346200	22.92693100	17.14052700
C	8.21802200	19.90249200	15.14964200
H	7.44623500	19.62457500	14.41326100

H	9.01892100	20.41483600	14.59337600
C	7.43783100	20.73034300	19.31968700
H	6.82089100	21.17150200	20.11962300
H	6.83282600	19.95268700	18.82643600
C	11.40439100	17.23989300	21.01252800
H	11.16477400	16.66682700	21.92312500
H	12.12162700	18.02681900	21.29593500

CaTHF

Final Single point energy: -4534.976960836433

Ca	4.61364300	10.15897400	13.85832400
O	4.45268200	8.65271900	15.65859500
O	4.86795300	10.91946500	11.63478800
N	6.72684600	9.44241500	14.58557000
N	2.77274000	8.71441900	13.60733500
C	7.87754900	10.05406700	14.06420800
C	7.98935500	8.47575100	16.49162800
H	8.92493500	8.83699100	16.07804500
C	0.62170500	9.57029300	12.79366700
C	6.80878200	8.75799300	15.76628700
C	1.78186200	8.78310500	12.60747400
C	8.29483300	11.31368300	14.55644000
C	-0.38628400	9.56074300	11.82857300
H	-1.26307800	10.18997400	11.96977100
C	2.50926800	7.81654100	14.61901700
C	7.96871800	7.73182700	17.67224400
C	-0.29794400	9.84014400	15.16216700
C	5.54511500	7.51552200	17.48641900
C	5.61085400	8.28616400	16.34223400
C	0.51047000	10.45056500	14.02757900
H	1.53756700	10.52691300	14.41609800
C	1.43254900	6.90130500	14.65879200
H	0.74573100	6.90137400	13.82122700
C	0.08347200	11.88488100	13.71778700
C	9.33978400	11.99497500	13.94053900
H	9.64904600	12.96232200	14.33150100
C	3.22710000	6.92307200	16.80971300
C	1.93790800	8.08985500	11.38273900
C	9.24740200	7.44745800	18.47105400
C	9.60679100	10.20764800	12.36810800
H	10.12458200	9.77473100	11.51462100
C	9.99667900	11.46479200	12.82643700
C	-0.28505900	8.79433700	10.66978900
C	8.57725600	9.48753300	12.97699900
C	1.25649700	6.00310800	15.71039400
C	0.48128600	12.49839800	12.52359400
H	0.99541800	11.91026000	11.77032900
C	-1.62990900	9.45568600	14.99374800
H	-2.09956900	9.53826400	14.01730500
C	0.89850100	8.08597600	10.45453400
H	1.01985100	7.53332900	9.52533800
C	0.27552400	9.72122000	16.42947700
H	1.31882900	9.99511400	16.56879200
C	0.09955300	4.99282600	15.72537800
C	3.38109100	7.76285400	15.72171200
C	2.15174800	6.02665800	16.79021100
H	2.00831400	5.34782200	17.62239100
C	3.56675800	7.20365100	9.62368700
C	6.74716700	7.23426600	18.14918500
H	6.72734400	6.64416800	19.05765900
C	7.55484300	11.87421600	15.76825800
H	7.50147100	11.05900500	16.50147200
C	8.96951800	7.01206500	13.33239900
C	-0.59547500	12.66210800	14.66138000
H	-0.91519300	12.21418600	15.59775300
C	6.12006800	12.23053200	15.43158100
C	8.21852300	8.07572700	12.54023300
H	7.15835500	7.94671600	12.79047100
C	3.24971200	7.35738700	11.11092100
H	4.04028100	7.99918200	11.52818800
C	0.21650900	13.84254700	12.28216500
H	0.53599500	14.29314500	11.34585300
C	3.33651200	6.04909500	11.87419200
C	-0.86454600	14.00859100	14.42080900
H	-1.39542500	14.59009600	15.16996300
C	4.16517700	7.11030300	18.00297500
C	-2.37238500	8.97738900	16.07015300
H	-3.40804900	8.68316000	15.92120800
C	10.26409200	7.20448200	13.81572400
H	10.75404200	8.16527000	13.67862300
C	5.79631400	12.92471600	14.25878700
H	6.58985100	13.20602800	13.57129700
C	-0.46303800	9.24650900	17.50988500
H	0.00401600	9.16018700	18.48753100
C	8.30589300	13.00215100	16.45726200
C	-0.77723000	5.08692300	14.47051200
H	-1.25058700	6.07190400	14.38175600
H	-1.57298200	4.33591600	14.52791300
H	-0.19830700	4.89756900	13.55939000
C	3.96320000	5.99299100	9.05240000
H	4.03515000	5.10238200	9.66841700
C	9.47534400	5.92590000	18.55225600
H	8.64331900	5.42122100	19.05343700
H	10.39255400	5.70843100	19.11319400
H	9.57679800	5.50049900	17.54726200
C	-1.79442600	8.87834500	17.33439600
H	-2.37537500	8.50585900	18.17374100
C	10.93093800	6.17969200	14.48498400
H	11.94087300	6.34519300	14.85116100
C	-0.79590900	5.24611000	16.95280700
H	-0.23522900	5.14281300	17.88762500
H	-1.62320500	4.52572600	16.97249200
H	-1.21721500	6.25622900	16.91869600
C	-0.45807400	14.60742600	13.23207200
H	-0.66828900	15.65674800	13.04476000
C	5.08212600	11.86868900	16.30223900
H	5.31723500	11.31637900	17.20959800
C	10.49026800	8.08427800	17.83837200
H	10.67323600	7.69853100	16.83003800
H	11.36803400	7.85298500	18.45204800
H	10.39910400	9.17503400	17.77994900
C	-1.41101200	8.73952600	9.67202200
H	-2.07927200	7.89489600	9.88276700
H	-1.03379000	8.60971200	8.65283500
H	-2.01585700	9.65093200	9.70526600
C	2.38909400	5.04125800	11.68074800
H	1.55921400	5.21031000	10.99748600
C	11.08646300	12.24014900	12.13556800

H	10.66454900	12.98557700	11.44950400
H	11.73090000	11.57951500	11.54838300
H	11.70793700	12.78020900	12.85715400
C	4.47028300	13.24038800	13.95799100
H	4.24112600	13.78768400	13.04798600
C	9.09713100	8.01653300	19.89559300
H	8.92289800	9.09845900	19.86003900
H	10.01148000	7.83398500	20.47314600
H	8.26089600	7.55521900	20.43004200
C	3.51083200	8.33066200	8.79333200
H	3.20123100	9.28208200	9.21384700
C	8.34895200	7.84489100	11.04391100
C	3.75466600	12.16399200	15.99386100
H	2.96272900	11.85513800	16.67062900
C	3.44035600	12.85150700	14.81664300
H	2.40659900	13.08294100	14.57503700
C	9.55223200	7.45442300	10.44870500
H	10.42726100	7.28030000	11.06982800
C	0.66466300	3.56147700	15.80920200
H	1.30466800	3.34917000	14.94662100
H	-0.15461600	2.83210500	15.82187900
H	1.26035200	3.41830800	16.71643300
C	8.35221800	5.77592100	13.54536700
H	7.34420200	5.61418900	13.17007600
C	9.63816000	7.27348800	9.07062700
H	10.58273500	6.97164600	8.62583300
C	2.50325000	3.82427600	12.34473300
H	1.76165700	3.04702800	12.17943000
C	8.03146600	14.35307500	16.24297800
H	7.22444300	14.64707000	15.57810000
C	10.30581700	4.95421200	14.69726600
H	10.82277700	4.16025900	15.22921100
C	4.27146100	11.94787700	9.54887600
H	3.64517000	11.59797900	8.72404300
H	4.30950700	13.04062700	9.50716200
C	3.81293300	8.24985600	7.43972500
H	3.75678300	9.14246300	6.82176500
C	4.38353400	5.82355000	12.76556200
H	5.10768400	6.61618100	12.94495800
C	6.08180100	11.35505300	10.96230800
H	6.87549300	10.65201100	11.22685300
H	6.35015100	12.36206000	11.31323800
C	9.34509900	12.65885600	17.32906400
H	9.56289600	11.60689800	17.50473000
C	4.26739400	5.90585200	7.69303500
H	4.56975300	4.94953800	7.27454600
C	4.18780000	7.02924700	6.87815100
H	4.42222200	6.96004200	5.81950600
C	3.55838800	3.60538600	13.22985200
H	3.64323400	2.65866600	13.75636000
C	4.49521000	4.61278600	13.44502100
H	5.31072800	4.45946800	14.14760800
C	9.00814700	4.75677500	14.22758600
H	8.50585400	3.80724800	14.39304500
C	5.69092700	11.36226200	9.49859300
H	6.37333900	11.95990900	8.88852900
H	5.67712700	10.33697000	9.11373100
C	8.78378400	15.33948100	16.88046500
H	8.55489000	16.38690900	16.70336500
C	4.23224400	5.85838400	18.88121100
H	4.87759000	6.02964000	19.74698200
H	4.61655900	4.99845900	18.32231000
H	3.24122800	5.60806800	19.26986700
C	10.09717400	13.63995000	17.96506200
H	10.89859800	13.35308200	18.64053200
C	9.81902400	14.98797900	17.74107000
H	10.40198900	15.75736100	18.23954700
C	8.51711900	7.46584700	8.26545700
H	8.58119100	7.31395000	7.19142200
C	3.61193400	8.28302000	18.85273500
H	2.60756700	8.03964000	19.21835400
H	3.54963500	9.19950600	18.25570400
H	4.26825000	8.47006300	19.71053200
C	3.73067700	11.49097100	10.91312700
H	3.32978200	12.32950900	11.49405500
H	2.96934900	10.70638300	10.85329300
C	7.22964300	8.02532100	10.22722300
H	6.27821500	8.30256300	10.67817000
C	7.30907900	7.83805700	8.85022400
H	6.42000900	7.96731700	8.23939500

ClCaCl_anion

Final Single point energy: -5223.292043417916

Ca	10.83698800	15.61553800	6.05795600
O	11.66763700	16.89584600	4.23418900
Cl	10.54058500	13.30369300	7.33533200
Cl	9.53248100	17.53818800	7.36421000
N	13.18001900	16.05292600	6.21423700
N	9.56496100	15.33501900	4.06195900
C	14.00048500	15.60606300	7.26331400
C	15.05997500	17.44587900	5.40077800
H	15.68732600	17.08794600	6.20861300
C	12.94875900	17.42753400	4.26485300
C	10.89171400	17.07694200	3.09899800
C	8.70579100	14.25075800	3.84709500
C	13.73726500	16.94911700	5.34322300
C	15.55740500	18.35139400	4.46363200
C	14.09359500	16.32273800	8.47899700
C	14.71845700	18.79238900	3.43474900
H	15.08700500	19.51134900	2.71134200
C	11.21724800	17.98785000	2.11334000
C	7.44804700	14.17619500	4.49032200
C	13.86348100	18.86276900	8.33416300
C	13.39894600	18.32631400	3.31716400
C	15.16244300	19.18735900	8.73039400
H	15.75748300	18.45517600	9.27036500
C	9.76341900	16.21982200	3.03937600
C	8.92444600	16.37942600	1.91475700
H	8.05182400	15.73812900	1.85683300
C	9.18226700	17.32890600	0.92558600
C	12.61028900	17.54112200	10.09969600
C	13.12365200	19.81067300	7.62322000
H	12.11478700	19.56136200	7.30015000
C	6.65379300	13.03763400	4.35136000
H	5.69434400	13.00017700	4.86519200
C	6.28173100	16.41314700	4.42890200
C	4.74393000	15.21308200	6.59940900
H	4.23511000	15.75113200	5.80468200

C	13.21188000	17.54202200	8.69818400
H	12.36617400	17.42695200	8.00689100
C	14.69752900	14.37791200	7.16196100
C	14.95390300	21.37937400	7.73769100
H	15.37807800	22.35249400	7.50470800
C	14.66160700	12.01710100	6.24057800
C	15.27020200	13.96842000	4.73482400
C	6.11005100	14.95022200	6.49439200
C	7.05863600	11.94534500	3.58652500
C	14.47365700	13.49998700	5.93717400
H	13.41380000	13.62799800	5.67089800
C	13.66365900	21.05799500	7.32175200
H	13.07582100	21.77955600	6.76017800
C	15.72048900	14.72973200	9.34722900
C	6.95746000	15.36726100	5.29979100
H	7.84868500	15.85761500	5.71256700
C	15.70272800	20.43720900	8.43993700
H	16.71569900	20.67347300	8.75610500
C	14.94599500	15.87829400	9.49102000
H	14.98625200	16.43185800	10.42813100
C	10.33301800	18.11794700	1.02931600
H	10.54196000	18.86450900	0.27107100
C	6.74081900	14.26715700	7.54224500
H	7.80710200	14.05703400	7.47510500
C	15.55682200	13.97725100	8.18374400
H	16.09307700	13.03538000	8.08428300
C	10.50727400	13.13835200	2.43943900
H	11.08447700	13.89765700	2.98597000
C	9.12838100	13.13296800	3.08111600
C	12.47848500	18.84329300	2.21234200
C	8.30731400	12.01241100	2.96846200
H	8.66744900	11.15153600	2.40580200
C	12.79079300	18.57587500	11.01695500
H	13.39317200	19.43824000	10.74617300
C	11.81675200	16.44846300	10.47528500
H	11.66366300	15.63520500	9.76815200
C	17.00104600	18.87213000	4.52019300
C	15.52928000	11.19402100	5.52329400
H	16.12165100	11.61025000	4.71403200
C	17.79008100	18.28263200	5.69580900
H	17.85794000	17.19083100	5.62660800
H	17.33117800	18.54027200	6.65690500
H	18.80926000	18.68593300	5.68827400
C	16.63944300	14.22588800	4.83203700
H	17.13398200	14.12569400	5.79576400
C	14.64591300	14.11866800	3.49642600
H	13.57737000	13.92720500	3.41307000
C	10.52920000	13.55575200	0.97879700
C	8.21273400	17.56982800	-0.24004300
C	12.20247500	18.51802900	12.28221200
H	12.35796300	19.33459300	12.98275900
C	11.22844800	11.81049500	2.65677300
C	6.55661100	17.76527400	4.64675000
H	7.28295900	18.04043300	5.40901600
C	5.36230600	16.06712600	3.43612000
H	5.15247400	15.01802100	3.24182700
C	9.51792500	13.21123100	0.08143900
H	8.63338300	12.69389300	0.44312300
C	4.02146900	14.79449000	7.71823400
H	2.95740200	15.00832800	7.77975100
C	11.41948300	17.42797400	12.64489600
H	10.95838300	17.38517500	13.62793700
C	13.89761100	11.44347700	7.26641500
H	13.20305700	12.06943100	7.82113900
C	16.68417200	14.29759300	10.42069600
H	16.38807000	14.68810600	11.39927800
H	17.69727700	14.66583300	10.21311900
H	16.74255300	13.20628900	10.48636000
C	11.22554200	16.39103900	11.73027700
H	10.60826800	15.53687700	11.99611400
C	4.65640400	14.11313700	8.75104700
H	4.09472200	13.79146500	9.62397700
C	11.54467300	10.93291200	1.61868800
H	11.28255000	11.18999100	0.59633900
C	17.37122200	14.61259900	3.71395400
H	18.43653900	14.80825900	3.80668000
C	15.64127900	9.83579300	5.82657300
H	16.32205300	9.21330900	5.25147400
C	6.02475700	13.85335900	8.65850500
H	6.53681700	13.32962400	9.46169700
C	4.71690200	17.05112400	2.69139800
H	4.00127000	16.76468900	1.92479400
C	4.99538400	18.39742300	2.91686600
H	4.50075600	19.16498200	2.32749900
C	12.07456100	20.29859100	2.54435200
H	12.96443600	20.93312600	2.62505500
H	11.53542600	20.33555500	3.49717200
H	11.42371800	20.70398100	1.76132200
C	7.11418600	16.50244500	-0.31903600
H	6.48188600	16.50305200	0.57486300
H	7.53947800	15.49969200	-0.44115100
H	6.47150200	16.70783000	-1.18295800
C	11.58837100	11.45725000	3.96324000
H	11.34747100	12.13008700	4.78537700
C	15.37095300	14.52162700	2.37729100
H	14.86835200	14.64672200	1.42160400
C	5.92407300	18.75104600	3.89352300
H	6.15976400	19.79776400	4.06797400
C	16.73820100	14.76531200	2.48146600
H	17.30536600	15.08091600	1.60983300
C	13.22225600	18.82193300	0.86096800
H	12.58674400	19.20387000	0.05728700
H	13.52457500	17.79963400	0.60825000
H	14.11777200	19.44866000	0.89418000
C	7.54124400	18.94348600	-0.04424900
H	6.82630600	19.14075200	-0.85356700
H	8.28495200	19.74770000	-0.03950200
H	7.00134600	18.97282800	0.90908400
C	17.73744900	18.50048100	3.21820100
H	18.77116200	18.86732700	3.25070500
H	17.24819500	18.93888300	2.34238500
H	17.75929300	17.41368300	3.08528100
C	16.99873100	20.40579800	4.66589300
H	16.48010700	20.70390000	5.58290700
H	16.49938800	20.88891800	3.81971200
H	18.02841900	20.78273300	4.71244700
C	14.88561900	9.27949200	6.85224100
H	14.97152500	8.22206300	7.08787000

C	6.20542300	10.70882500	3.47774100
H	6.24842400	10.28249600	2.46990100
H	5.16000900	10.92788400	3.71546900
H	6.54614200	9.93124800	4.17341600
C	11.64725000	14.23999900	0.49292500
H	12.43246500	14.52891400	1.18806400
C	12.19850300	9.72728900	1.87872800
H	12.43471200	9.05746900	1.05568000
C	8.96831400	17.56890600	-1.58210200
H	9.47545000	16.61047400	-1.73610300
H	9.71993300	18.36283700	-1.62823900
H	8.26432300	17.72625700	-2.40876400
C	14.00809100	10.09304700	7.57152800
H	13.40127500	9.67022900	8.36822100
C	12.24236500	10.25958900	4.22375600
H	12.52728500	10.01395200	5.24289400
C	12.55033600	9.38608500	3.18020200
H	13.06662600	8.45158600	3.38415000
C	9.62831500	13.52921700	-1.27088500
H	8.82929700	13.25439600	-1.95489900
C	11.76006300	14.56446300	-0.85473700
H	12.63377000	15.10547300	-1.20941700
C	10.75144900	14.20102100	-1.74612800
H	10.83489000	14.45236700	-2.80010300

ClCaCl

Final Single point energy: -7758.493779677996

Ca	10.88968400	15.59661600	5.99777900
P	6.10069300	19.53358400	11.29220900
P	7.00401400	9.66146600	8.99025200
O	11.76506800	16.74944200	4.13349300
Cl	10.65651600	13.43833800	7.54156400
Cl	9.61148500	17.66691500	7.10655100
N	13.20674700	16.07026300	6.21719100
N	9.63120900	15.24249600	4.01074600
C	14.01571900	15.60080100	7.26408700
C	15.03804400	17.56104700	5.46926000
H	15.64413700	17.25723500	6.31498900
C	12.99672800	17.38131200	4.22328900
C	10.97764100	16.94449600	3.00974000
C	8.72190100	14.18946800	3.86956300
C	13.75598700	16.97949700	5.35393000
C	15.52512000	18.47934100	4.53829000
C	14.04133000	16.23508800	8.52809800
C	14.71584300	18.84213600	3.45712000
H	15.07426600	19.56797200	2.73481200
C	11.29811300	17.85530300	2.02258200
C	7.47679700	14.20926100	4.54508600
C	13.82383600	18.78185000	8.55806800
C	13.43876400	18.28578500	3.27873000
C	15.12844100	19.04782300	8.97772900
H	15.72241200	18.25453400	9.42422900
C	9.83062000	16.11018600	2.97173400
C	5.17424400	19.27064100	9.76327400
C	8.97439500	16.28507800	1.86370900
H	8.08427800	15.66636000	1.82499500
C	9.23276300	17.22984500	0.86890900
C	12.46824500	17.34963200	10.14378300
C	13.09310700	19.80969100	7.95447900
H	12.08500800	19.60461500	7.59831100
C	6.63978500	13.09349600	4.51191300
H	5.69029400	13.13102800	5.04264900
C	6.30197600	16.42631400	4.29595500
C	4.91527000	15.44812700	6.69208000
H	4.31955400	15.75681800	5.83786400
C	13.14896600	17.43882100	8.78107300
H	12.34594200	17.38096200	8.03519200
C	14.75301100	14.40017800	7.11263500
C	14.93901800	21.33877700	8.23369300
H	15.37317900	22.32668000	8.10560100
C	14.79308800	12.09919100	6.07830500
C	15.37927400	14.12712400	4.66371200
C	6.29032300	15.25927100	6.54646700
C	9.95823400	19.83792000	10.06491100
H	10.68999200	19.18570000	9.60362900
C	6.97644400	11.94127900	3.80406100
C	14.58000400	13.58853300	5.83416800
H	13.52310900	13.71613500	5.55872700
C	13.64439700	21.07719000	7.78979300
H	13.06392800	21.86024200	7.30863700
C	15.65867500	14.61445000	9.36556100
C	7.03967300	15.48959000	5.23976400
H	7.96012300	16.01756500	5.51583400
C	3.77612800	19.19504700	9.82313600
H	3.25427300	19.31970700	10.76808200
C	15.68021000	20.31723500	8.82301000
H	16.69765300	20.50643000	9.15568000
C	14.85203100	15.73464600	9.54878200
H	14.83880700	16.22522700	10.52105900
C	5.17547600	20.71425400	12.29945800
C	10.40038400	17.99577800	0.95193700
H	10.61575600	18.73421000	0.18663400
C	7.03043200	14.88647400	7.67680200
H	8.10349000	14.73102600	7.58879400
C	15.57218600	13.94553400	8.14411900
H	16.13369400	13.02335900	8.00650500
C	10.41785600	12.95527700	2.44365200
H	11.05531000	13.68426900	2.96107300
C	9.07322400	13.01169000	3.15340800
C	8.05956600	21.51286300	11.24149200
H	7.32590000	22.16661300	11.70247500
C	12.57645900	18.68726800	2.08404300
C	8.20267300	11.92377800	3.13491600
H	8.49415400	11.02309400	2.59654200
C	12.84259200	18.13028900	11.23834800
H	13.65637500	18.84332200	11.13866500
C	3.05079200	18.97346700	8.65839900
H	1.96746000	18.91614400	8.70471200
C	4.63058000	21.84905600	11.68537300
H	4.73098900	21.99853500	10.61351400
C	11.40397200	16.45186200	10.29824500
H	11.09751100	15.83566000	9.45501500
C	16.91780000	19.11093800	4.67093800
C	6.26394700	17.98435100	12.20802100
C	15.82959200	11.36403100	5.50371800
H	16.52426400	11.84991400	4.82498100
C	7.74643000	20.18078800	10.95049800
C	8.39292400	9.40791600	7.86984500

C	8.70038400	19.33609900	10.36923700
H	8.47339500	18.29592700	10.14928900
C	9.43437800	8.56164200	8.27231700
H	9.38674200	8.03863100	9.22299000
C	3.71159200	18.83308500	7.44037700
H	3.14420800	18.66062100	6.52998100
C	17.70892300	18.54541600	5.85728000
H	17.85430400	17.46296000	5.76307600
H	17.20690100	18.74484700	6.81029500
H	18.69732200	19.01770300	5.89222000
C	16.73029800	14.45507000	4.79160500
H	17.21465500	14.35941600	5.76105800
C	5.83816700	19.12828200	8.54118600
H	6.92009700	19.19294100	8.47903500
C	14.76782100	14.27670200	3.41800100
H	13.71167400	14.03613600	3.30994600
C	10.38722200	13.37359700	0.98001900
C	8.24842800	17.49593800	-0.27887800
C	12.17034000	18.02187600	12.45565100
H	12.47753500	18.64024000	13.29516600
C	10.27419900	21.16272500	10.35310400
H	11.26498100	21.54210000	10.11707600
C	6.76098600	8.12212900	9.91034000
C	10.53429600	8.39201200	7.44282500
H	11.34114700	7.73305000	7.74905300
C	11.11804200	11.60595000	2.56566700
C	10.60023100	9.06491900	6.22544300
H	11.46175500	8.93164400	5.57925800
C	6.64471200	17.78013300	4.27733800
H	7.47048400	18.12462700	4.89722800
C	9.57093500	9.91669800	5.83438700
H	9.63495500	10.45510400	4.89299000
C	5.09955300	18.91139000	7.38403600
H	5.61569400	18.79855300	6.43633100
C	5.49320500	10.07580800	8.08513600
C	5.26652900	15.98840700	3.46604000
H	5.00578300	14.93324800	3.44295100
C	7.38778600	11.01388000	10.12189400
C	5.04008200	20.51895500	13.67604600
H	5.45508700	19.63583500	14.15262500
C	3.95542400	22.78644900	12.45688300
H	3.53233900	23.66693200	11.98301400
C	7.32254000	17.82590200	13.10975800
H	8.09069600	18.58900200	13.20067300
C	9.29998700	13.11864000	0.14473300
H	8.38968900	12.69586800	0.56267700
C	8.46097800	10.09306300	6.65350800
H	7.66498000	10.76426400	6.34167100
C	4.29437900	15.26773200	7.92873100
H	3.22170500	15.42137900	8.01654800
C	11.10397600	17.13915700	12.59310700
H	10.57147800	17.06510000	13.53733000
C	5.27372300	11.40419100	7.70265800
H	5.98661700	12.18401600	7.95777000
C	13.90151200	11.43879900	6.93467200
H	13.08019500	12.00036400	7.37538400
C	9.32836500	21.99748100	10.94306200
H	9.57495600	23.02940800	11.17378000
C	16.57686300	14.12650100	10.45451700
H	16.21831200	14.43320800	11.44200000
H	17.58778500	14.53590600	10.33092100
H	16.66497300	13.03537400	10.44098200
C	10.72178100	16.35344000	11.50550000
H	9.88076900	15.66949500	11.59568300
C	5.04148500	14.91009700	9.04524000
H	4.56010400	14.77631200	10.01033200
C	10.91515100	10.57151100	1.64628400
H	10.23173600	10.71684700	0.81376800
C	17.45774100	14.90869600	3.69507400
H	18.50930200	15.15830900	3.81101000
C	15.98480200	10.00597300	5.78972700
H	16.79996200	9.45203700	5.33141900
C	6.41842300	14.72334400	8.91342200
H	7.01794000	14.44922700	9.77772600
C	3.81925800	22.59397100	13.83062600
H	3.28671200	23.32765900	14.42887700
C	4.56666600	16.88877500	2.66672600
H	3.76132400	16.53101400	2.03035300
C	8.68216900	11.53775000	10.16764200
H	9.44890700	11.18624900	9.48467800
C	6.37236000	6.92806200	11.96701600
H	6.23776300	6.93423000	13.04431500
C	4.90449800	18.24051200	2.66992600
H	4.36590700	18.94080800	2.03707200
C	6.34479600	5.72764900	11.26364900
H	6.18398000	4.79277700	11.79263800
C	12.20512800	20.18193600	2.21256800
H	13.10781400	20.80087500	2.25485900
H	11.62661100	20.35104200	3.12717500
H	11.60361300	20.50641500	1.35655300
C	4.35918000	21.46348100	14.43762600
H	4.24756900	21.31092000	15.50675200
C	7.07990800	16.50295000	-0.29076000
H	6.48600400	16.56903600	0.62673700
H	7.43149200	15.47110600	-0.40265000
H	6.41921600	16.73090800	-1.13512700
C	6.53393600	5.72050100	9.88286700
H	6.52325100	4.78423400	9.33323400
C	12.02886600	11.39951700	3.60495800
H	12.19395000	12.18934900	4.33482000
C	6.58067300	8.12883800	11.29543100
H	6.61371100	9.05834900	11.85451000
C	15.48667300	14.74652600	2.32204000
H	14.98933500	14.87196300	1.36342500
C	6.74651400	6.91235000	9.20213200
H	6.91174800	6.89822900	8.12788400
C	5.95437800	18.68190200	3.47153700
H	6.24255200	19.73002300	3.46618200
C	16.83718600	15.06036000	2.45625000
H	17.40072600	15.42898600	1.60334300
C	13.37710400	18.47179400	0.78060400
H	12.78616100	18.76485500	-0.09238400
H	13.65027100	17.41596900	0.67393400
H	14.29462300	19.06790700	0.77992200
C	7.67132700	18.91619300	-0.11563500
H	6.95224200	19.13078600	-0.91654300
H	8.46256500	19.67236700	-0.15401600
H	7.15515700	19.01055600	0.84625300

C	17.73490100	18.85082900	3.39065100
H	18.73569200	19.29046500	3.48496700
H	17.25595700	19.28829700	2.50915300
H	17.84470100	17.77489000	3.21711900
C	16.76952100	20.63156500	4.87106000
H	16.18414000	20.84329900	5.77275200
H	16.26307700	21.09721400	4.01913900
H	17.75580100	21.10046400	4.97987500
C	5.28435000	16.99553200	12.08290900
H	4.47191000	17.10699500	11.37148200
C	15.10373900	9.36363100	6.65298800
H	15.22544500	8.30717200	6.87673000
C	3.19589100	10.74280500	6.66873900
H	2.29700400	11.00504000	6.11806300
C	6.06193800	10.74446600	3.77505300
H	5.99670000	10.31887200	2.76794200
H	5.05325500	11.01253800	4.10331200
H	6.42107000	9.94576800	4.43822200
C	4.12056200	11.72993800	6.99719800
H	3.94883800	12.76282700	6.71179800
C	11.53825200	13.94488000	0.42819200
H	12.38706300	14.15668200	1.07608200
C	11.59886100	9.36425700	1.76653100
H	11.42466400	8.57364100	1.04134200
C	8.96670800	17.40349900	-1.63760100
H	9.39195900	16.40464300	-1.78003900
H	9.77798400	18.13361000	-1.72030700
H	8.25700000	17.59705900	-2.45160900
C	14.05588300	10.08888600	7.22297200
H	13.35332600	9.59779700	7.89115800
C	4.56134900	9.08308000	7.76252900
H	4.71329400	8.05449300	8.07269200
C	12.73575600	10.20470500	3.71244400
H	13.45638200	10.08025000	4.51550800
C	7.38420200	16.68108900	13.89632900
H	8.20379100	16.55610100	14.59750500
C	8.98354400	12.53799700	11.08686100
H	9.98568600	12.95550800	11.11169500
C	12.52047900	9.17944100	2.79473600
H	13.07189300	8.24642400	2.87684400
C	5.35605200	15.85668200	12.87610200
H	4.59354900	15.08935100	12.78167000
C	6.39109500	11.50238600	10.97745500
H	5.37654100	11.11518600	10.92500100
C	9.36978800	13.40607700	-1.21732400
H	8.51466000	13.19846100	-1.85558400
C	3.41716800	9.42168500	7.04973300
H	2.69360100	8.65119300	6.80143000
C	11.60721600	14.24436600	-0.92746000
H	12.50704500	14.69722700	-1.33585400
C	6.39948300	15.70239000	13.78534800
H	6.44992300	14.81238700	14.40670100
C	8.00500700	13.00176000	11.95984800
H	8.24756600	13.78023000	12.67775500
C	10.52433500	13.96284900	-1.76003900
H	10.57623000	14.19052600	-2.82129500
C	6.70955100	12.48817600	11.90176600
H	5.94119800	12.85956300	12.57247800

ClCaTHF_anion

Final Single point energy: -4995.342156230235

Ca	4.98630900	9.06205400	12.87159300
Cl	5.78730900	7.61762600	10.79211700
O	4.82944000	7.86185600	14.89750600
O	4.83704200	11.01058100	11.54491100
N	6.91367300	9.37989200	14.24044700
N	2.73659100	8.34064000	13.30354600
C	7.98739500	10.25984300	13.98977500
C	8.09335200	8.67647000	16.29502400
H	8.94277100	9.29034200	16.02029300
C	0.66656600	9.54617800	12.72759200
C	6.99105200	8.66408900	15.40733000
C	1.58124100	8.49072400	12.50248200
C	8.06812200	11.51204700	14.64741000
C	-0.54286000	9.58353300	12.03243100
H	-1.23971500	10.39589400	12.22936700
C	2.55043300	7.50843500	14.38366400
C	8.12534100	7.91251500	17.46079700
C	0.58773700	10.23264300	15.15289000
C	5.89624700	7.06325300	16.93345600
C	5.90058500	7.83854300	15.78871800
C	0.99882500	10.62859100	13.74497400
H	2.09681400	10.70137500	13.76287800
C	1.32765700	6.87859300	14.71614400
H	0.47977300	7.06987400	14.07096900
C	0.48920200	12.01228800	13.34209000
C	9.13598400	12.36978200	14.39287100
H	9.18924900	13.31948100	14.92191900
C	3.53385500	6.42147500	16.37012800
C	1.29164800	7.57547300	11.46225600
C	9.31968700	7.94323700	18.42580600
C	10.06555100	10.80735800	12.84573000
H	10.84626400	10.52650700	12.14166500
C	10.14803500	12.03801800	13.49186400
C	-0.87233500	8.62800400	11.07364200
C	9.01103700	9.92091900	13.07400200
C	1.18706800	6.03921700	15.81812100
C	0.63775000	12.44727000	12.01889300
H	1.02985300	11.76002500	11.27622000
C	-0.75322200	10.01328500	15.47968700
H	-1.51516800	10.09422200	14.70768800
C	0.07929400	7.65462700	10.77737700
H	-0.11898700	6.94650500	9.97460300
C	1.54890000	10.10681500	16.15463500
H	2.59701700	10.23976500	15.90018800
C	-0.15185600	5.37656400	16.17315000
C	3.63398000	7.23920700	15.25868200
C	2.29730600	5.81509800	16.63604800
H	2.20892100	5.15778300	17.49386500
C	2.40303600	6.32099400	9.56986800
C	7.02523200	7.10843700	17.76577100
H	7.04002600	6.49572600	18.66033300
C	6.97620900	11.90677600	15.63203600
H	6.60332200	10.97911900	16.07776500
C	9.39556700	7.44402300	13.31555300
C	-0.03921400	12.91327300	14.26934900
H	-0.16524500	12.60911000	15.30420800
C	5.78169700	12.57096900	14.97041200

C	8.96964700	8.56424500	12.38475600
H	7.91600200	8.36935900	12.14698200
C	2.31434000	6.51758600	11.07982700
H	3.28986500	6.92059700	11.37918800
C	0.27760400	13.73416700	11.63685700
H	0.40571000	14.04328300	10.60257100
C	2.15717100	5.21536100	11.84302200
C	-0.40245500	14.20580100	13.89086300
H	-0.80902700	14.88614800	14.63465500
C	4.73203000	6.13876600	17.26914400
C	-1.12447600	9.70561300	16.78440600
H	-2.17216700	9.54116300	17.02303600
C	10.61727700	7.48521300	13.99098300
H	11.25910600	8.35690800	13.88030400
C	5.90076900	13.42220100	13.87171600
H	6.87634000	13.57350800	13.41673400
C	1.18363200	9.79694600	17.46271000
H	1.94850900	9.70270700	18.22923200
C	7.51283900	12.73925800	16.78952800
C	-1.25194800	5.69966500	15.15410300
H	-1.45193800	6.77651300	15.10653200
H	-2.18045000	5.19767700	15.44922500
H	-0.98474000	5.35371100	14.14886600
C	2.45770600	5.06415300	8.96636400
H	2.38721100	4.16892900	9.57682200
C	9.87592800	6.51900000	18.61862700
H	9.11815600	5.84234000	19.02574900
H	10.72355100	6.53621400	19.31491200
H	10.22077500	6.10868300	17.66377400
C	-0.15678300	9.60420400	17.78372300
H	-0.44646800	9.36264900	18.80285800
C	11.01964500	6.42274700	14.79459200
H	11.97563900	6.46646000	15.31031200
C	-0.62032100	5.87241000	17.55487000
H	0.10676400	5.62558400	18.33564400
H	-1.57677800	5.40405700	17.81938200
H	-0.75548200	6.95858200	17.54649800
C	-0.24525100	14.62452900	12.57381600
H	-0.52815000	15.63115800	12.27840600
C	4.51725100	12.37986200	15.53541000
H	4.41792500	11.72439900	16.39891700
C	10.46446500	8.83182600	17.92255400
H	10.84599500	8.48684800	16.95508700
H	11.29002400	8.79958100	18.64247200
H	10.15604700	9.87778600	17.81607400
C	-2.20405400	8.65541900	10.37166400
H	-2.93949000	8.03648800	10.90156200
H	-2.12425600	8.26468700	9.35230000
H	-2.60696800	9.67181400	10.32321000
C	0.95760700	4.49967100	11.84003100
H	0.09431000	4.89905700	11.31301500
C	11.27856600	12.99198600	13.21083900
H	11.00543600	13.70625000	12.42343400
H	12.17232700	12.45891600	12.87235700
H	11.53769000	13.57351200	14.10138200
C	4.78165400	14.07285900	13.35292800
H	4.89245500	14.73311800	12.49625600
C	8.85535100	8.48114400	19.79415300
H	8.44145700	9.49146000	19.69795000
H	9.70104500	8.52165900	20.49188600
H	8.08266700	7.84076200	20.23162000
C	2.51175500	7.45251900	8.74999800
H	2.47043900	8.43889200	9.20536700
C	9.69725800	8.53552300	11.04543300
C	3.39982600	13.02480600	15.01910300
H	2.42446800	12.85944500	15.46705600
C	3.52694900	13.87607700	13.92230200
H	2.64954500	14.37098500	13.51400000
C	10.66000200	7.57947900	10.71839300
H	10.94903600	6.83286500	11.45157400
C	0.01612700	3.84659500	16.23056700
H	0.34349900	3.45726700	15.26155000
H	-0.93878700	3.37324100	16.49129500
H	0.75488100	3.55140500	16.98270500
C	8.57437500	6.32797100	13.47804500
H	7.61526900	6.29812300	12.96483700
C	11.25684200	7.56557900	9.45622500
H	12.00521900	6.81128500	9.22721800
C	0.85899500	3.27636200	12.49545200
H	-0.08112800	2.73057500	12.48132700
C	7.47581200	14.13489400	16.80818700
H	7.01747900	14.67361500	15.98278800
C	10.19493000	5.30893000	14.94740600
H	10.50518300	4.48147900	15.57990500
C	4.43428800	11.03446400	9.19768500
H	4.23254200	10.05159600	8.76473400
H	4.05579100	11.79615400	8.51087100
C	2.66448000	7.33341000	7.37506100
H	2.75025500	8.22759900	6.76272700
C	3.24979500	4.68759500	12.53269000
H	4.18409400	5.24526600	12.55168900
C	6.00157600	11.62682400	10.94332800
H	6.88201900	11.28077200	11.49510600
H	5.91502800	12.71580600	11.05464800
C	8.08649600	12.07186100	17.87588500
H	8.10142400	10.98432000	17.86884900
C	2.60623200	4.93993800	7.58356700
H	2.64384300	3.94978200	7.13670400
C	2.70926800	6.07081100	6.78149900
H	2.82652500	5.97361900	5.70562700
C	1.95845100	2.75355700	13.17507900
H	1.87955600	1.80092200	13.69205900
C	3.15336800	3.46797300	13.19858700
H	4.01336300	3.07596100	13.73568200
C	8.96634800	5.26808200	14.29247700
H	8.31156200	4.40903400	14.41451100
C	5.94797200	11.19961000	9.47999900
H	6.42098000	11.94150700	8.83082200
H	6.45712200	10.24159100	9.34895200
C	8.01708800	14.84488400	17.87926700
H	7.98062400	15.93118100	17.87646200
C	5.18533300	4.67611300	17.04988700
H	6.04246100	4.43928000	17.69012500
H	5.47984000	4.52331000	16.00573200
H	4.36991600	3.98287200	17.28415800
C	8.62707300	12.77610200	18.94634300
H	9.06692000	12.23570800	19.78093900
C	8.59720000	14.17026200	18.95042800

H	9.01486300	14.72523000	19.78599100
C	10.89645700	8.50365100	8.49564400
H	11.35929300	8.49091700	7.51268000
C	4.32579200	6.32723900	18.74662900
H	3.51011900	5.65216400	19.01873200
H	3.99592500	7.35683000	18.92254700
H	5.16334700	6.11292100	19.41568700
C	3.77271700	11.17791500	10.57623100
H	3.33927700	12.17756900	10.71506300
H	3.00937200	10.42128900	10.79093900
C	9.34139200	9.47211100	10.06551300
H	8.59775300	10.22731300	10.30315000
C	9.92907900	9.45996400	8.80743100
H	9.63103300	10.19729500	8.06636600

ClCaTHF

Final Single point energy: -6262.940403124924

Ca	4.93974500	9.17439300	12.92275300
P	8.50919800	4.35068100	7.91649800
Cl	5.69974200	7.75600400	10.81366200
O	4.80682000	7.92517400	14.93058600
O	4.76275000	11.04699000	11.48897500
N	6.94466900	9.34315200	14.19102500
N	2.70746600	8.39240600	13.35123600
C	8.01572800	10.23820400	13.98438900
C	8.17601600	8.53680800	16.17377300
H	9.04364800	9.10684200	15.86555600
C	0.62924900	9.53883700	12.68847000
C	7.03423800	8.59618900	15.33947600
C	1.56243700	8.48671500	12.52714000
C	8.08556900	11.44572100	14.72389200
C	-0.56369300	9.53104300	11.96532600
H	-1.27314200	10.34422200	12.10692700
C	2.51638500	7.60054100	14.46049600
C	8.21894600	7.76790200	17.33528200
C	0.42747200	10.31426700	15.07978100
C	5.91976800	7.05902700	16.91584800
C	5.91833900	7.82776100	15.76578400
C	0.91789200	10.65552500	13.68088100
H	2.01405900	10.71741600	13.75417900
C	1.28534200	7.00660100	14.82345500
H	0.43390800	7.19929500	14.18356000
C	0.44872200	12.03409800	13.21706400
C	9.16060400	12.31279500	14.55663700
H	9.20204100	13.22666200	15.14680600
C	3.50395500	6.54277400	16.45726000
C	1.29861700	7.50951400	11.53609500
C	9.46136400	7.71963900	18.23540900
C	10.11022700	10.86322300	12.91575700
H	10.90015100	10.63527900	12.20344800
C	10.19272400	12.03672100	13.65845500
C	-0.86486900	8.52420600	11.05022500
C	9.04560500	9.96747800	13.05611500
C	1.13849900	6.20526800	15.95204900
C	0.58753100	12.41089400	11.87580300
H	0.93043800	11.67909600	11.15199300
C	-0.93451100	10.15202900	15.34640900
H	-1.65544700	10.23241900	14.53621400
C	0.09605200	7.53993200	10.82998600
H	-0.08786700	6.78681500	10.06574600
C	1.33292400	10.19572900	16.13344600
H	2.39645900	10.28187800	15.92818300
C	-0.20733400	5.57110000	16.33106200
C	3.60589400	7.33523500	15.32779200
C	2.25574500	5.97727200	16.75932300
H	2.16818200	5.34355500	17.63534700
C	2.51639700	6.16780100	9.74772400
C	7.08859500	7.03050000	17.69170400
H	7.10399400	6.41956400	18.58793300
C	6.95611600	11.79036600	15.68292500
H	6.57361500	10.84532300	16.08161000
C	9.37400000	7.45925500	13.04279100
C	-0.02154400	12.99358500	14.11856100
H	-0.14112100	12.73540200	15.16664700
C	5.78599400	12.46500700	14.98755900
C	8.99670300	8.68468300	12.23206000
H	7.94749600	8.54306600	11.94236800
C	10.11552200	4.39520300	8.75356400
C	2.33052500	6.43197100	11.24009600
H	3.29130600	6.83681400	11.58418000
C	0.27772400	13.69857100	11.45154500
H	0.39639700	13.96136800	10.40341600
C	2.11245200	5.15406200	12.03388100
C	-0.33395300	14.28544300	13.69771400
H	-0.69490700	15.01083800	14.42213400
C	8.67469500	3.30657600	6.45288500
C	4.70679400	6.24218700	17.34238500
C	-1.38031400	9.90736400	16.64125800
H	-2.44361300	9.78780400	16.83255700
C	10.55912100	7.40766300	13.78026400
H	11.20738200	8.28110300	13.81240400
C	5.95009400	13.34492000	13.91648400
H	6.94452000	13.51313800	13.51087500
C	0.89276600	9.95357500	17.43267800
H	1.61499500	9.86603800	18.24029300
C	7.44355900	12.58307700	16.88820600
C	-1.32645700	5.94330600	15.35000400
H	-1.49184200	7.02641200	15.31865100
H	-2.26135800	5.46758300	15.66732200
H	-1.10172000	5.59891000	14.33375100
C	2.85438900	4.90169400	9.26142600
H	2.92048800	4.06263800	9.94654100
C	9.97287800	6.26941900	18.33231800
H	9.21386400	5.60563700	18.75847300
H	10.86333400	6.22273500	18.97152300
H	10.23887600	5.88876000	17.33997300
C	11.28311700	4.45171500	7.98098700
H	11.22976500	4.42927500	6.89596200
C	-0.46794000	9.81752300	17.69202100
H	-0.81686300	9.63172300	18.70425000
C	10.91529400	6.25400700	14.47283300
H	11.84386500	6.22814800	15.03745100
C	-0.62559200	6.04271400	17.73669000
H	0.10905200	5.74847100	18.49320300
H	-1.59112000	5.59981400	18.01098500
H	-0.72364700	7.13280100	17.76278500
C	7.25783300	3.66740800	9.01743100
C	10.19431200	4.40130000	10.14929300

H	9.30111300	4.34901200	10.76269600
C	-0.18373600	14.64694500	12.36253100
H	-0.42743300	15.65338400	12.03353800
C	4.49709900	12.25287200	15.48739800
H	4.36195800	11.57545700	16.32914000
C	10.60556500	8.59614100	17.71013100
H	10.93944400	8.27426600	16.71760800
H	11.45966800	8.52322400	18.39272800
H	10.31444400	9.65118000	17.64886800
C	-2.18067000	8.50654500	10.31877100
H	-2.93252000	7.93506300	10.87796800
H	-2.08175900	8.03894200	9.33413400
H	-2.57396500	9.51900400	10.18458700
C	0.98234200	4.35442700	11.84304900
H	0.21053000	4.67034300	11.14553000
C	11.34007900	12.99592100	13.48441700
H	11.03465900	13.87635300	12.90499000
H	12.17391000	12.52445000	12.95607500
H	11.70444200	13.35812500	14.45174500
C	4.85338300	14.00633700	13.36519100
H	5.00061400	14.69009200	12.53294700
C	9.09174400	8.21337500	19.64808700
H	8.71312300	9.24128900	19.61307500
H	9.97445200	8.19548200	20.29925900
H	8.32060200	7.58458500	20.10403200
C	2.45716200	7.22625300	8.83186200
H	2.20758300	8.22307100	9.18558000
C	8.97919600	6.90465900	6.93894900
H	10.03334800	6.64579500	6.96250300
C	9.78894700	8.80987700	10.93471300
C	3.40240200	12.91186500	14.93910700
H	2.40921900	12.73963500	15.34260200
C	3.57501200	13.79177000	13.87182700
H	2.71525400	14.29686800	13.43864100
C	11.43812500	4.47066500	10.76732600
H	11.49122100	4.48088800	11.85263800
C	8.00911500	6.00996800	7.40411900
C	10.89730300	8.02145100	10.62656000
H	11.21858700	7.24892700	11.31690000
C	-0.07518000	4.03641600	16.34229300
H	0.20055000	3.66627500	15.34942100
H	-1.02944900	3.57815100	16.63106600
H	0.68883300	3.70426100	17.05300300
C	8.54095900	6.33959800	13.03447700
H	7.60474800	6.38535300	12.48183600
C	8.06274400	3.68040500	5.25369200
H	7.52258500	4.61985900	5.17994100
C	9.37684400	2.09864600	6.54727100
H	9.85514100	1.80989100	7.47960400
C	12.59841600	4.53238500	10.00160200
H	13.56783100	4.58575000	10.48887300
C	11.61398300	8.22096200	9.44462600
H	12.47590500	7.59356300	9.23237000
C	6.73160000	2.38978400	8.80591600
H	7.03087300	1.80109000	7.94427100
C	0.84517000	3.14498300	12.51797900
H	-0.03824700	2.53303400	12.35470300
C	7.33948000	13.97150400	16.98317000
H	6.86178200	14.53259100	16.18412200
C	10.07762800	5.13965700	14.45745000
H	10.34901800	4.24356000	15.00927400
C	4.34831600	10.91993400	9.14982200
H	4.19355100	9.89519500	8.80164600
H	3.92404800	11.60385300	8.40982300
C	2.70225300	7.02106900	7.47875300
H	2.63772300	7.85888200	6.78860400
C	9.46061000	1.26832300	5.43677700
H	10.00486500	0.33145900	5.50668400
C	3.08512000	4.72720100	12.93794400
H	3.94767300	5.36316900	13.12233600
C	5.90949800	11.65846800	10.85285400
H	6.80078400	11.34244800	11.40525500
H	5.81046800	12.74959800	10.93003000
C	8.04801400	11.88338900	17.93785300
H	8.12135800	10.79959700	17.86942200
C	12.52004500	4.52213800	8.61036200
H	13.42438500	4.56447800	8.01082000
C	3.11488500	4.69433900	7.90719000
H	3.37841000	3.69813700	7.55971000
C	3.03345400	5.75134600	7.00615100
H	3.22811000	5.59123900	5.94893400
C	8.15544300	2.84145500	4.14789600
H	7.68475300	3.13155100	3.21351700
C	6.84884800	4.43192700	10.11621900
H	7.21410900	5.44483100	10.26149000
C	8.85152000	1.63917000	4.23899200
H	8.92364900	0.98848100	3.37226300
C	1.83765400	2.71583700	13.39859100
H	1.73119900	1.77056700	13.92406100
C	8.58838800	8.14435200	6.44967900
H	9.34053000	8.83850700	6.08968300
C	2.95593700	3.51654700	13.61421300
H	3.72719200	3.20289600	14.31339600
C	8.88372600	5.18900500	13.74102000
H	8.21603700	4.33063500	13.73165700
C	5.85341300	11.18385800	9.40098200
H	6.26894900	11.93567800	8.72423200
H	6.41729500	10.25534300	9.28244300
C	7.24210200	8.50062200	6.44131600
H	6.94213800	9.47717100	6.07149900
C	7.84173000	14.64623100	18.09587000
H	7.75303400	15.72797700	18.15295900
C	5.05319900	4.73935500	17.22360100
H	5.90469000	4.48789500	17.86517700
H	5.31483200	4.49275300	16.18842300
H	4.19933800	4.12115800	17.52098900
C	5.41718700	2.62372800	10.81642800
H	4.69204700	2.22247700	11.51948100
C	6.65518600	6.36194300	7.39199800
H	5.89459700	5.67772900	7.75705900
C	8.54921300	12.55266300	19.04870400
H	9.01350800	11.98935500	19.85435800
C	5.93757500	3.90000800	11.01661100
H	5.62250500	4.49493200	11.86676900
C	6.28061100	7.61317900	6.91472400
H	5.23181700	7.89186300	6.92560500
C	5.80616100	1.87524200	9.70878700
H	5.38911800	0.88661100	9.54256200

C	8.44991000	13.94166100	19.13089900
H	8.83732800	14.46845800	19.99862100
C	11.23249200	9.21269400	8.54929700
H	11.79305700	9.37056900	7.63170300
C	4.35630200	6.56999900	18.81067300
H	3.49952600	5.98087600	19.14944900
H	4.10770600	7.63196100	18.91264300
H	5.19598300	6.34679800	19.47483400
C	3.69138500	11.13433800	10.51933800
H	3.23666600	12.13097600	10.60007600
H	2.94549100	10.37584000	10.78209000
C	9.40048700	9.78788700	10.00911600
H	8.54265300	10.41533600	10.23350000
C	10.11269700	9.99428400	8.83583800
H	9.79135000	10.76411500	8.13896500

Cl_anion

Final Single point energy: -460.342687195893

Cl	16.07104000	0.83903000	12.51927000

FBiphenyl

Final Single point energy: -601.737268733443

C	0.37267800	0.20552700	0.01515200
C	1.71469100	0.25420400	-0.38874600
C	2.41818900	1.45115600	-0.37222100
C	1.80247200	2.63314300	0.04661800
C	0.46622200	2.59016000	0.45099100
C	-0.23956900	1.39433700	0.43670600
H	2.21884600	-0.65919300	-0.69191100
H	3.46186100	1.46819500	-0.67753000
H	-0.02725500	3.50388600	0.77401700
H	-1.28370200	1.38531100	0.73671500
C	-0.37636500	-1.06915400	0.00345500
C	-0.18071800	-2.00692000	-1.02017900
C	-1.29967800	-1.36704000	1.01557400
C	-0.88786500	-3.20453100	-1.03084700
H	0.51217700	-1.78584300	-1.82767000
C	-2.00392900	-2.56626300	1.00449400
H	-1.44945300	-0.66457800	1.83104900
C	-1.80200400	-3.48999800	-0.01878700
H	-0.72992400	-3.91420000	-1.83832100
H	-2.70797200	-2.78342600	1.80308000
H	-2.35313000	-4.42611600	-0.02765800
C	2.54472300	3.92904600	0.01220300
H	3.62090700	3.78830900	0.15481800
H	2.15528400	4.64400900	0.74376800
F	2.38157000	4.53170600	-1.27065200

FCa_anion

Final Single point energy: -4402.566487600167

Ca	10.82571400	15.52225300	6.07387600
O	11.37627100	17.22924600	4.50938900
F	9.73505600	15.48691700	7.85272700
N	13.12163400	16.03061600	6.14576700
N	9.52167300	15.34036500	4.13256000
C	13.95355800	15.64276800	7.20740400
C	14.97374800	17.31263200	5.11152400
H	15.68629600	16.81375800	5.75902400
C	12.71797000	17.60463300	4.38452000
C	10.61008100	17.32144100	3.34080400
C	8.76449100	14.20267200	3.81733200
C	13.61328500	16.95545800	5.25924200
C	15.40247200	18.23552700	4.15848200
C	14.14654400	16.49032100	8.32786800
C	14.45087700	18.87234600	3.34732000
H	14.76945300	19.60292400	2.61376700
C	10.86483300	18.31538600	2.41370300
C	7.49154200	13.99513000	4.39833100
C	14.25054400	19.02796800	7.96052600
C	13.08871500	18.57127500	3.46738700
C	15.61294600	19.14591600	8.23799500
H	16.13583400	18.32552100	8.72212100
C	9.63932400	16.31236800	3.17347900
C	8.84929900	16.41727200	2.00470800
H	8.08400400	15.66396300	1.85687100
C	9.03927400	17.42815700	1.06444900
C	12.78605300	18.03327700	9.76400400
C	13.60487600	20.08852800	7.31801500
H	12.54450400	20.00260800	7.08807700
C	6.76340500	12.84675200	4.09219800
H	5.78595900	12.70320300	4.54948800
C	6.35152000	16.24094300	4.63799100
C	4.62096000	14.60571300	6.36322400
H	4.16637400	15.21019700	5.58344400
C	13.42465400	17.82899500	8.39319200
H	12.59774500	17.75465800	7.67454200
C	14.52570800	14.34993200	7.24630100
C	15.65694500	21.35510700	7.26008700
H	16.20307400	22.25381700	6.98640200
C	14.24227300	11.93969000	6.55348700
C	15.20824600	13.62440600	4.91627100
C	6.00590900	14.44123800	6.39378100
C	7.26051600	11.86787600	3.23053100
C	14.27583800	13.39055400	6.09197400
H	13.26883600	13.61501000	5.71164300
C	14.29951600	21.24065200	6.96458900
H	13.78136400	22.05002000	6.45684700
C	15.55512400	14.81684800	9.40607000
C	6.94525800	15.04381900	5.35806500
H	7.80808400	15.42607300	5.91906500
C	16.31040600	20.30217300	7.89474300
H	17.37175300	20.37628600	8.11778000
C	14.93463100	16.06526800	9.39661100
H	15.04311100	16.71582500	10.26316900
C	10.06313400	18.36599000	1.26715900
H	10.22924200	19.14955100	0.53757900
C	6.56489700	13.66974500	7.42020900
H	7.64544300	13.54715600	7.45990500
C	15.31611100	13.96484300	8.32876200
H	15.74417500	12.96394400	8.33874400
C	10.74666200	13.27772600	2.53148100
H	11.23315800	13.98535900	3.22067700
C	9.30643500	13.17407900	3.00775800
C	11.97492300	19.31495300	2.73015700
C	8.54800400	12.03845900	2.72387900
H	8.99012800	11.24669500	2.12051200
C	13.30145400	18.90689300	10.72215000
H	14.17863800	19.50535000	10.49095500

C	11.64508700	17.28591300	10.08107700
H	11.22140500	16.60737300	9.34120700
C	16.89169100	18.53524300	3.93754700
C	15.18152200	10.98973000	6.15669600
H	15.98137500	11.27412700	5.47898700
C	17.78471300	17.88559500	5.00234400
H	17.70977100	16.79328000	4.98206600
H	17.52386700	18.23211500	6.00886400
H	18.83020000	18.15258300	4.81043700
C	16.56357000	13.90971400	5.08941100
H	16.96497300	14.01841500	6.09409600
C	14.70772700	13.51202900	3.61760400
H	13.65266000	13.29249400	3.47246100
C	10.93193500	13.86859200	1.14624900
C	8.12481100	17.57456700	-0.16041900
C	12.69918000	19.02346000	11.97522600
H	13.11648700	19.70717800	12.70997600
C	11.48808600	11.95117300	2.69086700
C	6.60709700	17.52754300	5.11702000
H	7.25842900	17.65426200	5.97985900
C	5.52650600	16.09287800	3.52117300
H	5.33606400	15.09790200	3.12530400
C	10.11603600	13.51359800	0.07135000
H	9.26480400	12.85776200	0.23533800
C	3.81131400	14.00411900	7.32750900
H	2.73418300	14.14363000	7.28618700
C	11.56818000	18.27411900	12.28375100
H	11.09640500	18.36885500	13.25804600
C	13.21411200	11.54305900	7.41761800
H	12.47523200	12.27709000	7.73486400
C	16.44281800	14.39779500	10.54747000
H	16.15623000	14.90007800	11.47666800
H	17.49087400	14.65472900	10.34640200
H	16.39813200	13.31622000	10.70938500
C	11.04052300	17.40596900	11.32738100
H	10.15146800	16.82208700	11.55158100
C	4.37610900	13.23431700	8.33921500
H	3.74564900	12.76972400	9.09243300
C	12.15998800	11.32245200	1.64226400
H	12.14165500	11.76108000	0.64910100
C	17.40161400	14.06307400	3.98721800
H	18.45526200	14.28313100	4.13848800
C	15.09971700	9.67362300	6.61425700
H	15.84051600	8.94679100	6.29133000
C	5.76126100	13.07183300	8.38351800
H	6.21581700	12.48192100	9.17515700
C	4.95286100	17.20452000	2.90946600
H	4.30953000	17.07195500	2.04340100
C	5.21352000	18.48408900	3.39462800
H	4.77582200	19.35266500	2.91009200
C	11.40371300	20.38342100	3.69748900
H	12.18864400	21.09775100	3.97287500
H	11.02353500	19.91768100	4.61229400
H	10.58193600	20.92563300	3.21548300
C	7.16328400	16.38937100	-0.31745800
H	6.48349300	16.30516300	0.53695700
H	7.70917700	15.44440500	-0.42025900
H	6.55578500	16.53176700	-1.21826900
C	11.54358500	11.36496400	3.96213700
H	11.02728400	11.84321400	4.79289000
C	15.53862800	13.67634300	2.51318200
H	15.12471100	13.59335800	1.51110200
C	6.04926100	18.64309800	4.49818900
H	6.26857100	19.63777000	4.87729700
C	16.89307700	13.94809500	2.69525600
H	17.54643100	14.07781700	1.83671100
C	12.48711600	20.02294900	1.47450800
H	11.67899400	20.57880900	0.99093400
H	12.90421200	19.31242000	0.75259700
H	13.26039000	20.75038200	1.73718600
C	7.28691400	18.85889900	-0.00024100
H	6.61386700	18.98399500	-0.85792800
H	7.92888000	19.74393600	0.06356400
H	6.68105400	18.81005500	0.91144100
C	17.30468900	17.98296200	2.55867800
H	18.37233800	18.16289100	2.37995600
H	16.73646900	18.46248100	1.75453600
H	17.12235300	16.90322300	2.50799700
C	17.14908200	20.05309300	3.96739900
H	16.84850100	20.47447100	4.93247200
H	16.59960900	20.57712200	3.17949200
H	18.21730700	20.25406200	3.81983500
C	14.07574200	9.29013000	7.47329900
H	14.00999400	8.26460700	7.82631000
C	6.43968900	10.65693800	2.87515700
H	5.84383300	10.83582500	1.97086900
H	5.74300800	10.39962300	3.67904700
H	7.07772200	9.78960900	2.67818400
C	12.01036200	14.72627900	0.91525000
H	12.64663400	15.01987400	1.74842200
C	12.86748500	10.13817200	1.85651600
H	13.38513800	9.66638500	1.02531200
C	8.95781000	17.68152300	-1.45071800
H	9.56011700	16.77890700	-1.59538300
H	9.63336900	18.54221800	-1.43192200
H	8.29289800	17.79610800	-2.31560900
C	13.12832000	10.23416700	7.87396600
H	12.31894500	9.94577200	8.53959100
C	12.25024100	10.18982000	4.17960400
H	12.29896400	9.76784500	5.17955400
C	12.91728100	9.56824000	3.12357600
H	13.47578200	8.65168900	3.29361400
C	10.38289400	13.99108600	-1.20937700
H	9.73707800	13.70592700	-2.03599200
C	12.27694100	15.21091100	-0.36179800
H	13.11703600	15.88233000	-0.52012600
C	11.46800800	14.83593300	-1.43247500
H	11.67328600	15.21115500	-2.43145800

FCaBr_looseBr

Final Single point energy: -6976.880358543852

Ca	11.06700100	15.80648400	6.26857100
O	11.58148300	17.30916100	4.51335200
F	10.04922500	16.84123600	7.76088900
N	13.39323500	16.27568900	6.18893300
N	9.71344000	15.42047600	4.36648000
C	14.30498900	15.93574900	7.20251900
C	15.17368700	17.58714800	5.06533200

H	15.91548600	17.16852700	5.73527700
C	12.90318500	17.72646400	4.34219900
C	10.78371000	17.30650700	3.36633900
C	8.89124800	14.29546500	4.22107300
C	13.83337000	17.16683900	5.24470500
C	15.54917900	18.48212100	4.06482000
C	14.48437400	16.78157600	8.32505300
C	14.56606700	19.01648600	3.21837900
H	14.84606600	19.72202000	2.44543400
C	10.99324000	18.23482200	2.36392200
C	7.66913300	14.20985800	4.93078500
C	14.20265700	19.28396000	7.89039200
C	13.22232300	18.64984000	3.36333100
C	15.54347500	19.63008800	8.06868000
H	16.20815100	18.94823000	8.59319200
C	9.80436400	16.29109300	3.31747400
C	8.98037800	16.29731500	2.16614500
H	8.20951000	15.53749000	2.10915100
C	9.13733900	17.23095200	1.14341100
C	13.17151400	18.19733100	9.93278500
C	13.37119400	20.16469700	7.19518900
H	12.32704300	19.89941800	7.04123600
C	6.87877000	13.06865700	4.82177000
H	5.94339600	13.01794600	5.37568000
C	6.80728200	16.58520600	5.00414500
C	4.92761700	15.34810900	6.89792400
H	4.53552900	15.96011200	6.09084600
C	13.61043900	18.01837400	8.48226100
H	12.69582500	17.81338300	7.90889000
C	15.00209000	14.70548600	7.18045000
C	15.19902300	21.70988300	6.89007400
H	15.58655600	22.64693600	6.49921200
C	14.90079000	12.26340900	6.55742900
C	15.44376900	13.98505900	4.78141600
C	6.27507300	14.98706900	6.90472500
C	7.26887100	11.97557700	4.04510700
C	14.70864400	13.69789900	6.07653900
H	13.63918700	13.80280700	5.84200800
C	13.86350700	21.36610500	6.69287500
H	13.20295400	22.03402100	6.14626600
C	16.18045200	15.28767100	9.23513000
C	7.26032800	15.38444400	5.81296800
H	8.16685300	15.71116600	6.34044900
C	16.03753400	20.83574900	7.57874400
H	17.08428500	21.08920600	7.72669400
C	15.41459500	16.44960800	9.30937300
H	15.52450400	17.10341100	10.17330000
C	10.15656000	18.19034200	1.24174400
H	10.28744300	18.91928200	0.45094200
C	6.75402500	14.21211200	7.96833500
H	7.80259200	13.91745200	7.98620300
C	15.93321500	14.41368500	8.17752400
H	16.46448500	13.46454900	8.13982600
C	10.69598900	13.17382700	2.83563500
H	11.24508400	13.98762500	3.33204200
C	9.31534200	13.17128100	3.47350400
C	12.07259800	19.29148800	2.58700900
C	8.50359700	12.03781700	3.40300200
H	8.86488500	11.16250100	2.86470000
C	13.57333900	19.26689000	10.73279000
H	14.22061900	20.03604400	10.32122100
C	12.32625600	17.22850400	10.48923700
H	11.99598800	16.39524800	9.87272300
C	17.01678600	18.87329700	3.83839600
C	15.84332300	11.39084300	6.01529300
H	16.48287300	11.72127700	5.20185800
C	17.95094500	18.29322200	4.90809600
H	17.93834000	17.19813000	4.90530000
H	17.67578600	18.63913500	5.91126100
H	18.97833000	18.61780100	4.70696900
C	16.78875900	14.35785900	4.76717600
H	17.31338800	14.50348800	5.70874000
C	14.78133900	13.81504200	3.56392800
H	13.73277600	13.52258500	3.56547000
C	10.72530100	13.49823900	1.35272500
C	8.20505900	17.26383400	-0.07601000
C	13.15165300	19.36192900	12.06032700
H	13.47851000	20.20236100	12.66734900
C	11.46190700	11.88902100	3.15201300
C	7.28948200	17.85480200	5.32794000
H	8.01928400	17.95430300	6.12943800
C	5.89384400	16.45968300	3.95562700
H	5.53061100	15.47186900	3.67994900
C	9.80803400	12.95590700	0.45161700
H	8.98439700	12.35201500	0.82191700
C	4.07473000	14.93557900	7.92311200
H	3.02801300	15.22802900	7.89954500
C	12.31622200	18.39225300	12.60393100
H	11.98464600	18.46816900	13.63596700
C	14.08231000	11.80145100	7.59491000
H	13.32599900	12.46178800	8.01397700
C	17.22190900	14.97459300	10.27651700
H	16.95380200	15.40524400	11.24650900
H	18.19884000	15.38819500	9.99438900
H	17.34804900	13.89440700	10.39982400
C	11.90081500	17.32338100	11.80806700
H	11.23979100	16.56335100	12.21624100
C	4.55864100	14.15978600	8.97147100
H	3.89476100	13.84153000	9.77082700
C	12.08929100	11.11329500	2.17587600
H	12.02064300	11.39933300	1.13053300
C	17.46023200	14.54657400	3.56202800
H	18.50776900	14.83700500	3.56793800
C	15.96961900	10.08795900	6.50164900
H	16.70872100	9.42210900	6.06331900
C	5.90694800	13.80062200	8.99015000
H	6.30205100	13.20013100	9.80567900
C	5.45015900	17.58285700	3.26248800
H	4.73480600	17.46953700	2.45179200
C	5.93505300	18.84652700	3.59329500
H	5.59902100	19.72245600	3.04467800
C	11.47078800	20.40770900	3.47846700
H	12.23136000	21.16765900	3.69296700
H	11.11639700	19.99469800	4.42853100
H	10.62463300	20.88342100	2.96859000
C	7.21963900	16.08869800	-0.09129600
H	6.55483400	16.10515500	0.77961300
H	7.74481100	15.12675400	-0.10651700

H	6.59557400	16.14903600	-0.99038300
C	11.57840400	11.49500300	4.49128800
H	11.09276800	12.07939200	5.27115700
C	15.44628700	14.01174000	2.35644500
H	14.91312700	13.87870500	1.41833200
C	6.86398200	18.97815000	4.62386800
H	7.25910000	19.95794900	4.87988600
C	16.79150500	14.37469100	2.35179300
H	17.31321500	14.52999100	1.41122800
C	12.54336700	19.91823200	1.27307900
H	11.70782600	20.39940500	0.75706200
H	12.98199900	19.16866900	0.60547000
H	13.28863000	20.69583100	1.46373500
C	7.39370000	18.57422900	-0.05681700
H	6.71668600	18.61464900	-0.91965900
H	8.05205200	19.44836700	-0.09735100
H	6.79459200	18.64169600	0.85760800
C	17.46961200	18.34281100	2.46368300
H	18.52414300	18.59085700	2.28812600
H	16.87586100	18.78111100	1.65462500
H	17.35687900	17.25404400	2.41665200
C	17.17249400	20.40566200	3.85712900
H	16.85869900	20.81112100	4.82450900
H	16.57318700	20.88534300	3.07709000
H	18.22206600	20.67914500	3.69120800
C	15.15368600	9.64044000	7.53521100
H	15.24925100	8.62497100	7.91034800
C	6.38824200	10.76015900	3.92300600
H	6.98060900	9.86103300	3.72658800
H	5.67397600	10.86946000	3.09649200
H	5.80720600	10.59897800	4.83649100
C	11.76413800	14.28840600	0.85271000
H	12.47512100	14.73291300	1.54661300
C	12.81067300	9.97050300	2.52706900
H	13.29105800	9.38138900	1.74991900
C	9.02822000	17.21018200	-1.37680600
H	9.62791800	16.29491000	-1.41613600
H	9.70572800	18.06546300	-1.46317600
H	8.35815300	17.22266600	-2.24562200
C	14.20382800	10.50619000	8.07966100
H	13.54661200	10.16762000	8.87660900
C	12.29447700	10.35833600	4.84246900
H	12.37855500	10.08181300	5.88971400
C	12.91597600	9.58733200	3.85952900
H	13.48021600	8.70045200	4.13560700
C	9.93677400	13.18123500	-0.91728300
H	9.21184700	12.75142800	-1.60395200
C	11.89647100	14.51726200	-0.51314000
H	12.70858000	15.13994400	-0.87982200
C	10.98652200	13.95457200	-1.40646800
H	11.08608500	14.13116200	-2.47415600
Br	10.20795100	12.23874200	8.24198600

FCaBr

Final Single point energy: -6976.899519459926

Ca	11.11866300	15.82684200	6.21692200
O	11.85526300	16.93110600	4.22174700
F	10.14660100	17.37648000	7.27044200
N	13.46605300	16.31692300	6.19605400
N	9.74171200	15.37950000	4.30715400
C	14.33343800	15.96306800	7.23841000
C	15.24133200	17.74943600	5.23516800
H	15.90747300	17.48862300	6.04916100
C	13.10464900	17.52950100	4.16548100
C	11.01076100	17.02804600	3.12778300
C	8.86273900	14.29687200	4.24329100
C	13.94916100	17.17541900	5.25116500
C	15.66267600	18.60653000	4.21823600
C	14.40861200	16.73155900	8.42260000
C	14.77769200	18.91442400	3.17955800
H	15.08835600	19.59259100	2.39190600
C	11.26625600	17.86586800	2.06001800
C	7.68332600	14.28148000	5.02898200
C	14.05112900	19.24766500	8.17723700
C	13.48376800	18.36866400	3.13608900
C	15.35425300	19.63348100	8.49761500
H	16.00403700	18.94239800	9.02848600
C	9.88231300	16.17028800	3.20332700
C	8.97593100	16.24396300	2.12223800
H	8.10156600	15.60483100	2.17092000
C	9.16730900	17.11718800	1.05090800
C	12.89422100	17.94037100	10.01823800
C	13.24108200	20.14424300	7.47559200
H	12.22812900	19.84714400	7.21108200
C	6.84517800	13.16967400	5.01358700
H	5.94449500	13.17822600	5.62520500
C	6.85470200	16.66713300	5.03711800
C	5.11946000	15.53446000	7.13329300
H	4.66084300	16.08502100	6.31709100
C	13.46885000	17.91351400	8.60605000
H	12.61802600	17.73209200	7.93516300
C	15.08893300	14.76669500	7.17135700
C	15.01320800	21.78147100	7.44615400
H	15.38850500	22.76037000	7.15968900
C	15.12868900	12.36228200	6.34784600
C	15.56798800	14.27054700	4.73493500
C	6.46823000	15.18444900	7.06313300
C	7.13859200	12.03680200	4.25149600
C	14.85837000	13.82216900	5.99745400
H	13.78188300	13.89062700	5.77872200
C	13.71682200	21.39971700	7.10747300
H	13.07512900	22.07936100	6.55274500
C	16.13481500	15.26260200	9.31702600
C	7.36302000	15.50789100	5.87432100
H	8.31140100	15.85482400	6.30459100
C	15.83075700	20.89215200	8.14024900
H	16.84831200	21.17600100	8.39692200
C	15.30112600	16.37249900	9.43388200
H	15.32901900	16.96400900	10.34810700
C	10.31792700	17.91250700	1.02495000
H	10.47925000	18.59773100	0.19938300
C	7.03437800	14.49186800	8.14096100
H	8.08809300	14.21908100	8.10133900
C	15.99019100	14.45519700	8.18744700
H	16.57132500	13.53764600	8.11606800
C	10.52210300	13.05519900	2.77763000
H	11.14221000	13.84664700	3.21967800
C	9.18817800	13.12946600	3.50669100

C	12.52675800	18.72421700	2.00101900
C	8.32948500	12.02990800	3.52740000
H	8.61510900	11.12774400	2.98775200
C	13.11790100	18.97746600	10.92328600
H	13.72496800	19.82887400	10.62877000
C	12.09633400	16.86142800	10.42211200
H	11.91192600	16.04603300	9.72428100
C	17.06879700	19.22427100	4.20563600
C	15.96341700	11.53816000	5.59264000
H	16.47763500	11.94043600	4.72499600
C	17.93007300	18.74214100	5.37949900
H	18.06314400	17.65426300	5.35730100
H	17.48729000	19.01595100	6.34355400
H	18.92129400	19.20617600	5.31939700
C	16.93140100	14.57294600	4.74394300
H	17.48147300	14.51967000	5.68100500
C	14.86945600	14.35643500	3.53057300
H	13.80385300	14.13299100	3.51585700
C	10.46943300	13.33387900	1.28518200
C	8.13383400	17.26416400	-0.07467600
C	12.56654200	18.93490200	12.20555900
H	12.75462900	19.75233100	12.89707900
C	11.23627600	11.73884600	3.07002100
C	7.37315800	17.94590200	5.25237100
H	8.17610600	18.07200000	5.97722800
C	5.85866700	16.49617200	4.07346700
H	5.46892800	15.49914000	3.87866300
C	9.38839700	12.96857400	0.48263200
H	8.50106900	12.54021900	0.94081000
C	4.35091200	15.19121800	8.24660400
H	3.30187800	15.47407600	8.28143600
C	11.77868300	17.85803000	12.59714700
H	11.34662500	17.82727900	13.59376200
C	14.46734400	11.80341100	7.45041600
H	13.79546400	12.42621400	8.03549400
C	17.14159300	14.92678400	10.38549500
H	16.84247100	15.33809100	11.35461500
H	18.12840700	15.34231400	10.14322700
H	17.26261400	13.84379100	10.49149100
C	11.54224000	16.81923300	11.69472400
H	10.92120700	15.97523700	11.98361700
C	4.92144200	14.49736600	9.30874200
H	4.32374400	14.23459300	10.17745600
C	11.29583200	10.68689300	2.15391400
H	10.83883600	10.79998000	1.17439200
C	17.58528900	14.94255900	3.57282800
H	18.64700200	15.17496100	3.59644700
C	16.14235900	10.19567800	5.93242300
H	16.79564100	9.57306400	5.32645000
C	6.27202600	14.15106000	9.25170800
H	6.73446200	13.61799900	10.07853600
C	5.36375900	17.58708500	3.36291500
H	4.58222100	17.43989500	2.62173400
C	5.87877700	18.86161700	3.59012900
H	5.49991900	19.71239200	3.02983200
C	12.13321700	20.21432700	2.12334700
H	13.02085200	20.85334400	2.05716600
H	11.64363000	20.40032800	3.08544400
H	11.44151800	20.49685700	1.32189100
C	7.00642200	16.22895100	0.02916800
H	6.44357500	16.33982000	0.96200800
H	7.39821300	15.20657800	-0.01832000
H	6.30715000	16.36523400	-0.80396600
C	11.84613800	11.57237200	4.31854500
H	11.80427600	12.38040000	5.04753800
C	15.51589600	14.74020500	2.35786700
H	14.95301400	14.81638500	1.43077300
C	6.89380800	19.03534900	4.52936000
H	7.31536000	20.02300800	4.69858800
C	16.87798300	15.03100800	2.37453200
H	17.38400000	15.33286300	1.46133800
C	13.23036100	18.49729600	0.64470300
H	12.57065200	18.76189900	-0.18685700
H	13.51633600	17.44495200	0.53730000
H	14.13181800	19.11128100	0.56245200
C	7.50652900	18.66989300	0.00485400
H	6.75630000	18.79974600	-0.78583200
H	8.26654000	19.44994400	-0.11195800
H	7.01664800	18.81472800	0.97414400
C	17.79507100	18.84811500	2.89945400
H	18.80275200	19.28236800	2.88969300
H	17.25823900	19.21741600	2.01981100
H	17.88576900	17.76033200	2.80887700
C	16.95712500	20.75858600	4.28781600
H	16.44489300	21.05674700	5.20879800
H	16.39404600	21.16254200	3.44007400
H	17.95534100	21.21524200	4.28295200
C	15.48814100	9.65508800	7.03357100
H	15.62587600	8.60982800	7.29722000
C	6.20240800	10.85753300	4.22397900
H	6.73363700	9.93735600	3.96118100
H	5.40562900	10.99963200	3.48207400
H	5.71818300	10.71135600	5.19509500
C	11.58995900	13.90643600	0.67480600
H	12.43289500	14.20740500	1.29411700
C	11.94145300	9.49403100	2.47960900
H	11.97554200	8.68649200	1.75261900
C	8.80869900	17.09538500	-1.44848800
H	9.28521900	16.11228300	-1.52379100
H	9.57433400	17.85804300	-1.62204000
H	8.06192300	17.18085000	-2.24789700
C	14.64474200	10.46877100	7.79191300
H	14.11516200	10.05845300	8.64805900
C	12.49590400	10.38698600	4.64382800
H	12.97509800	10.28579600	5.61368400
C	12.54539100	9.33982700	3.72385600
H	13.05668300	8.41443200	3.97601400
C	9.43272600	13.15455500	-0.89796400
H	8.58002100	12.86517200	-1.50709800
C	11.63568200	14.10153800	-0.70124000
H	12.51229300	14.55842600	-1.15344200
C	10.55749800	13.71546400	-1.49671700
H	10.58874100	13.86573900	-2.57256200
Br	10.98169600	13.48779000	7.88102300

FCaF_anion

Final Single point energy: -4502.579485547767

Ca	11.12027700	15.71474700	6.21909400

O	11.85223900	16.96885200	4.23630800
F	11.04303100	13.75224500	7.07594700
F	10.05778500	17.11091800	7.44108300
N	13.44961100	16.32556600	6.21171300
N	9.72111600	15.44252100	4.27715800
C	14.27910900	15.97673500	7.28043300
C	15.29133700	17.62495200	5.19481500
H	15.95682700	17.33097500	5.99831500
C	13.12454700	17.51402200	4.16429600
C	10.99758000	17.12268000	3.15794000
C	8.89451600	14.32847800	4.16654400
C	13.96632100	17.13193300	5.24404700
C	15.74212000	18.44910300	4.16352600
C	14.35881600	16.78415500	8.43986600
C	14.85077200	18.81420300	3.14895500
H	15.18257500	19.47351500	2.35396900
C	11.25878400	17.98235900	2.10901300
C	7.72533600	14.21657800	4.95594500
C	14.01423800	19.26672200	7.97108300
C	13.52640200	18.34315600	3.13461500
C	15.31315700	19.69225500	8.25669100
H	15.95642300	19.07035200	8.87488000
C	9.85508300	16.28047800	3.21233100
C	8.93237500	16.41294800	2.15120500
H	8.05174900	15.78104000	2.18672100
C	9.12224700	17.32447200	1.11236200
C	12.93570100	18.16761100	9.98789900
C	13.21138900	20.06536500	7.15442600
H	12.20359300	19.73275100	6.91341700
C	6.95441200	13.05662200	4.91162500
H	6.06322700	12.99044000	5.53426400
C	6.59452400	16.46858600	5.05666800
C	5.25901700	15.14863900	7.32681700
H	4.65612500	15.65168600	6.57556800
C	13.44049600	17.99274000	8.55962400
H	12.55455300	17.75396900	7.95402300
C	14.97104200	14.74227800	7.28125400
C	14.97916000	21.69450000	6.94842000
H	15.35461400	22.63334300	6.55003000
C	14.84655600	12.31645200	6.59254000
C	15.49458300	14.08971100	4.88750300
C	6.62232100	14.95708500	7.10336800
C	7.30311900	11.97128400	4.10633500
C	14.70905900	13.76452700	6.14228700
H	13.65031900	13.90230600	5.87968500
C	13.68950400	21.26770400	6.64016900
H	13.05380300	21.87169800	5.99788500
C	16.00272500	15.27754700	9.42336900
C	7.33504700	15.39491500	5.83452900
H	8.27012100	15.86748500	6.16231700
C	15.79080800	20.90014800	7.75627300
H	16.80406200	21.21818000	7.98894300
C	15.22294300	16.43226400	9.47709300
H	15.26764800	17.06245900	10.36435200
C	10.29049200	18.09365500	1.09564400
H	10.45504100	18.80451800	0.29269400
C	7.38104800	14.31693700	8.09231100
H	8.44724400	14.16553700	7.92715600
C	15.83112500	14.42501500	8.33141000
H	16.36075500	13.47383300	8.31251900
C	10.62515700	13.22560200	2.67821500
H	11.19881600	14.02734900	3.16586700
C	9.28242100	13.20470100	3.39095700
C	12.55947300	18.77721500	2.03508400
C	8.48673500	12.06014000	3.37328900
H	8.82297000	11.19516000	2.80189700
C	13.22473000	19.27788000	10.78091300
H	13.83737400	20.08109300	10.38189100
C	12.12943500	17.15603100	10.52750000
H	11.89014000	16.28803400	9.91649100
C	17.19090100	18.95537200	4.10096400
C	15.78277500	11.42801500	6.06587800
H	16.46627600	11.76003200	5.28974900
C	18.03451000	18.46166700	5.28312300
H	18.09057700	17.36726600	5.30714200
H	17.62650900	18.80669700	6.23991400
H	19.05514100	18.85069600	5.19070500
C	16.86876400	14.33525800	4.93221200
H	17.38108300	14.32228900	5.89184800
C	14.84595500	14.13229200	3.65208300
H	13.77224000	13.95703600	3.60747700
C	10.57263300	13.58382500	1.20388400
C	8.06074900	17.54461600	0.02610300
C	12.73246600	19.37177800	12.08426400
H	12.97152600	20.24529600	12.68552300
C	11.40265200	11.93593600	2.92758300
C	6.88857600	17.81287500	5.29897700
H	7.65954800	18.06261700	6.02545700
C	5.61708200	16.15662700	4.10936700
H	5.39378400	15.11397200	3.89590600
C	9.51740600	13.20925800	0.37155100
H	8.65674600	12.69799400	0.79439300
C	4.66196300	14.70300400	8.50721900
H	3.59774700	14.86044200	8.66338100
C	11.93800500	18.35945500	12.61095400
H	11.55164000	18.43424000	13.62384900
C	13.96419200	11.85072800	7.57702700
H	13.21050800	12.52908100	7.97150800
C	16.97672900	14.94424200	10.52273500
H	16.66475200	15.38383100	11.47543400
H	17.97796000	15.33302100	10.29542200
H	17.07101400	13.86161800	10.65554300
C	11.63465800	17.24853100	11.82182300
H	11.00626300	16.45426100	12.21630800
C	5.42245800	14.06478600	9.48164500
H	4.95839700	13.72168800	10.40245500
C	11.72432400	11.03154100	1.91491400
H	11.41903000	11.23704400	0.89265000
C	17.58174500	14.60318200	3.76732800
H	18.65096900	14.79266200	3.81955300
C	15.84529600	10.10770500	6.51626500
H	16.58043800	9.43028700	6.08912700
C	6.78916800	13.87553200	9.26936100
H	7.39568400	13.38569800	10.02682800
C	4.93966800	17.16499600	3.42797800
H	4.18086200	16.90470700	2.69429100
C	5.24317000	18.50248200	3.67231600
H	4.72548500	19.28930700	3.13010500

C	12.25136300	20.28249800	2.20458000
H	13.17090000	20.87380800	2.13002300
H	11.79817800	20.46953500	3.18428000
H	11.55562700	20.62329900	1.42964300
C	6.94118300	16.49679100	0.08325100
H	6.39469000	16.54164700	1.03105300
H	7.33878100	15.48236200	-0.03842600
H	6.22560500	16.68302800	-0.72598600
C	11.81463900	11.65241400	4.23692300
H	11.56972700	12.34904900	5.03958100
C	15.55214200	14.41517400	2.48560000
H	15.02881800	14.45843600	1.53371800
C	6.22405000	18.82332600	4.60895400
H	6.47706600	19.86327600	4.79859800
C	16.92487000	14.64635300	2.53880300
H	17.47730500	14.86960800	1.62998200
C	13.21090000	18.54676600	0.65333700
H	12.54267900	18.86453300	-0.15244100
H	13.43706200	17.48337800	0.51483800
H	14.14086700	19.11458700	0.55792200
C	7.43043100	18.93664400	0.23107200
H	6.65313000	19.12183200	-0.52158300
H	8.18486300	19.72658900	0.14920400
H	6.97278000	19.00525200	1.22495800
C	17.85413000	18.45865800	2.80167200
H	18.89324600	18.80799500	2.74770600
H	17.32494300	18.82758300	1.91695200
H	17.85362100	17.36400300	2.76493200
C	17.20972000	20.49556900	4.11019200
H	16.74241000	20.87702000	5.02366600
H	16.66695000	20.90827200	3.25364600
H	18.24300800	20.86290100	4.06710100
C	14.97189100	9.65794300	7.50029100
H	15.01862200	8.62963200	7.84867100
C	6.43862800	10.73962000	4.04179200
H	7.04024200	9.84231100	3.86355300
H	5.70699300	10.80793400	3.22587800
H	5.87766600	10.59984900	4.97129200
C	11.66021900	14.25798400	0.64014600
H	12.48123600	14.56899500	1.28371300
C	12.43938700	9.86697100	2.19980300
H	12.67983300	9.17492200	1.39655500
C	8.69358000	17.48080900	-1.37586500
H	9.15296400	16.50072100	-1.54475800
H	9.46429700	18.24540000	-1.51378100
H	7.92436900	17.63905100	-2.14213900
C	14.02633100	10.53894100	8.02891700
H	13.32660200	10.19669100	8.78712900
C	12.53074800	10.49551500	4.52032500
H	12.85456400	10.30025100	5.53878200
C	12.84651000	9.59534900	3.50154700
H	13.40982200	8.69299900	3.72498400
C	9.55157100	13.49442400	-0.99231300
H	8.71768900	13.19977500	-1.62456300
C	11.69723100	14.54872700	-0.71931000
H	12.54721400	15.08444400	-1.13453700
C	10.64248500	14.16050400	-1.54464000
H	10.66581900	14.38794900	-2.60707300

FcaF

Final Single point energy: -7037.787078533231

Ca	11.20600600	15.57687900	6.17727000
P	6.22718100	19.10023300	10.92341200
P	6.14262600	9.43029300	8.81183800
O	11.85757900	16.89674000	4.22912500
F	11.38035700	13.59579400	6.95273400
F	10.07993300	16.73523100	7.59018100
N	13.48916500	16.30870400	6.19523800
N	9.74138900	15.32526000	4.28698800
C	14.33562000	15.97817900	7.25689000
C	15.26054100	17.71843900	5.20348600
H	15.93461500	17.45453300	6.01027700
C	13.10559700	17.50245800	4.16223100
C	10.99243500	17.02468100	3.15339000
C	8.87329700	14.24197000	4.18582800
C	13.96392700	17.15492900	5.24027800
C	15.67383900	18.57008800	4.17947100
C	14.40592800	16.78350900	8.41753200
C	14.76981300	18.89205300	3.16159400
H	15.07164100	19.56936800	2.36986900
C	11.22640500	17.89308100	2.10388000
C	7.69460400	14.18758700	4.97517700
C	14.02168000	19.27696400	8.02781300
C	13.47160200	18.35411300	3.13767300
C	15.28039500	19.74361500	8.41165700
H	15.90573500	19.13094500	9.05653000
C	9.86621100	16.16103600	3.21586800
C	5.00144500	18.80646400	9.62563300
C	8.93790200	16.27341100	2.15670600
H	8.06756100	15.62846100	2.19745900
C	9.10579700	17.18235600	1.11230500
C	12.88126100	18.08144500	9.95311300
C	13.24395900	20.06871800	7.18045400
H	12.27189000	19.70186100	6.85649600
C	6.83755000	13.09627800	4.87884900
H	5.92665500	13.08477000	5.47578300
C	6.95391700	16.60166500	5.19634500
C	5.15934200	15.15765800	7.12415900
H	4.65805400	15.58326200	6.25954100
C	13.46017300	17.96788600	8.54676200
H	12.60715600	17.72836900	7.89439800
C	15.05573500	14.75886900	7.24775300
C	14.95046900	21.77233500	7.14258000
H	15.31250500	22.73766900	6.79914000
C	15.00781100	12.33715200	6.51527000
C	15.57950500	14.16687200	4.84212000
C	6.54360600	14.97803400	7.10299600
C	9.73670300	19.48663400	8.90617200
H	10.36062300	18.82789400	8.31033200
C	7.12437000	12.00442600	4.05346300
C	14.81752000	13.78893000	6.09694100
H	13.75099800	13.89245000	5.85322500
C	13.70197700	21.30652400	6.73703300
H	13.08538500	21.90493200	6.07118500
C	16.07999500	15.30469700	9.39150300
C	7.42276900	15.35030400	5.91884300
H	8.39016800	15.62480300	6.35609100
C	3.65474200	18.66303400	9.98835100

H	3.34896800	18.74967200	11.02756200
C	15.74079700	20.98307400	7.97615300
H	16.72323600	21.33241800	8.28345200
C	15.27946500	16.44429500	9.45168300
H	15.31255900	17.06965400	10.34295600
C	5.50459200	20.27853200	12.08804700
C	10.25637900	17.97670700	1.09114400
H	10.40521300	18.68629800	0.28406100
C	7.16084600	14.44550400	8.24284300
H	8.23998400	14.30363100	8.24144500
C	15.92321900	14.45411700	8.29470800
H	16.47463400	13.51549500	8.26833400
C	10.54646600	13.06204200	2.69497500
H	11.15503200	13.83280000	3.18668000
C	9.19955700	13.10765100	3.40023500
C	8.08093800	21.11780200	10.45788500
H	7.44523900	21.75378000	11.06574800
C	12.49512200	18.73731100	2.02936200
C	8.32766300	12.01853000	3.35202500
H	8.60818700	11.14322100	2.76765200
C	12.92222900	19.24977400	10.71322600
H	13.42119000	20.13094700	10.32048600
C	2.70118200	18.43034400	9.00536600
H	1.65780900	18.32218700	9.28606300
C	4.78852900	21.37450200	11.59118300
H	4.63739300	21.49589000	10.52174900
C	12.21791600	16.96690800	10.48445000
H	12.17432300	16.04995400	9.90083100
C	17.09346400	19.15450000	4.12961100
C	6.60700700	17.56819500	11.80491000
C	15.98815400	11.50027700	5.98305600
H	16.67095800	11.87998200	5.22847400
C	7.74822500	19.77739700	10.23667500
C	7.78718400	9.81372000	8.18493000
C	8.58281400	18.95509400	9.46709500
H	8.35145300	17.90604300	9.29817200
C	8.88845200	9.08003000	8.64444300
H	8.75145400	8.23031000	9.30726400
C	3.08239800	18.34861200	7.66741200
H	2.33329700	18.17143400	6.90068500
C	17.95589900	18.69512900	5.31182300
H	18.06853800	17.60488100	5.32683000
H	17.52649900	19.01065700	6.26954600
H	18.95538400	19.13695100	5.22793100
C	16.93922000	14.48332400	4.88335600
H	17.45721000	14.48388900	5.83998200
C	5.38331400	18.72559400	8.28426600
H	6.42122400	18.84320200	7.98969000
C	14.92344400	14.19133100	3.61002900
H	13.86052600	13.95894700	3.56669900
C	10.52476900	13.41792800	1.21779200
C	8.04727200	17.36680400	0.01620200
C	12.31647000	19.30744400	11.97023500
H	12.36026200	20.22981500	12.54383200
C	10.06889600	20.82196700	9.12457300
H	10.98134600	21.22676300	8.69470400
C	6.04928600	7.65518600	9.12812100
C	10.16771300	9.45510300	8.24913600
H	11.02521600	8.89004700	8.60280000
C	11.26090900	11.73525900	2.93719600
C	10.34900700	10.55507300	7.41383500
H	11.34730800	10.86459500	7.12211100
C	7.53948700	17.82826300	5.52200100
H	8.34161800	17.84447900	6.25876700
C	9.25124800	11.27699100	6.95209500
H	9.40176600	12.13867200	6.30959500
C	4.41868000	18.49537300	7.30914800
H	4.71923600	18.43020200	6.26766100
C	4.85581600	9.90823400	7.63559300
C	5.95496200	16.57087700	4.22133300
H	5.51755600	15.61789700	3.93081400
C	5.86634600	10.34885000	10.34406100
C	5.69628200	20.12111600	13.46285400
H	6.24714800	19.26857000	13.84938800
C	4.26840500	22.31004100	12.47667900
H	3.71258700	23.16060000	12.09397300
C	7.86251200	17.41210200	12.40330000
H	8.63503100	18.16543900	12.27597200
C	9.46074700	13.09725000	0.37417900
H	8.56678900	12.63828300	0.78790100
C	7.96796800	10.90889300	7.33442100
H	7.12291100	11.48290100	6.96914700
C	4.41221600	14.82562100	8.25381500
H	3.33644400	14.98306100	8.25120200
C	11.65712600	18.19682800	12.48486100
H	11.18386300	18.24190000	13.46261800
C	4.54057700	11.26520000	7.48813300
H	5.04143800	12.02348200	8.08518200
C	14.12960400	11.81164400	7.47347100
H	13.33738100	12.44899600	7.86080900
C	9.24599400	21.63387200	9.89985700
H	9.50981200	22.67216300	10.07728700
C	17.06346400	14.98469700	10.48620000
H	16.75654700	15.42996000	11.43784300
H	18.06076200	15.37679000	10.24809300
H	17.16507600	13.90366300	10.62634500
C	11.61155400	17.02150300	11.73174800
H	11.10116900	16.14326400	12.11806400
C	5.03851600	14.30945100	9.38424400
H	4.45848200	14.05911600	10.26856400
C	11.29183500	10.71164500	1.98735700
H	10.80560400	10.85606400	1.02604000
C	17.63017700	14.80677000	3.71915400
H	18.68815400	15.05158000	3.76885900
C	16.09763500	10.17276800	6.40277900
H	16.86718200	9.53680800	5.97276400
C	6.42026000	14.11781600	9.37335100
H	6.92200900	13.72426300	10.25336000
C	4.45681700	22.15431100	13.84893400
H	4.04446600	22.88598600	14.53767000
C	5.52700600	17.74647100	3.60713400
H	4.74488500	17.70847800	2.85310300
C	6.95953300	10.79094000	11.09429100
H	7.97382200	10.62739900	10.74209000
C	5.38728000	5.79891600	10.51194500
H	4.94821900	5.42103900	11.43020500
C	6.11326800	18.96568400	3.94042900
H	5.78874800	19.88013400	3.45105800

C	5.86284300	4.91546900	9.54693900
H	5.79217200	3.84426500	9.71210500
C	12.12493400	20.23071400	2.18194600
H	13.01888500	20.85900500	2.10115200
H	11.66327500	20.41003900	3.15934800
H	11.41680000	20.53390800	1.40282500
C	5.16844900	21.06315900	14.34003200
H	5.31183700	20.93994500	15.40916900
C	6.92367700	16.32586500	0.10823200
H	6.37880200	16.40343200	1.05528600
H	7.31605800	15.30635500	0.01833900
H	6.20779900	16.48843800	-0.70566800
C	6.43561700	5.39964200	8.37205000
H	6.81129900	4.71067000	7.62181200
C	11.91167300	11.53398500	4.16068600
H	11.89177800	12.31831100	4.91838900
C	5.47777700	7.17208500	10.30768000
H	5.11328100	7.85838100	11.06616000
C	15.60629000	14.52999900	2.44460600
H	15.07575100	14.55913100	1.49610300
C	6.53413000	6.76854400	8.15756800
H	6.99005800	7.14422300	7.24499500
C	7.12918400	19.00120900	4.89491500
H	7.60505100	19.94493900	5.15015500
C	16.96457900	14.83552800	2.49499700
H	17.49914500	15.10269800	1.58738400
C	13.16368500	18.52018100	0.65347000
H	12.48988100	18.80794600	-0.15888600
H	13.42880100	17.46488100	0.52377800
H	14.07323700	19.12022600	0.55961900
C	7.41992500	18.76741200	0.16070700
H	6.65185800	18.92456600	-0.60745600
H	8.17625300	19.55258400	0.05527600
H	6.95209200	18.87651400	1.14565400
C	17.78970700	18.70759600	2.82935700
H	18.80862600	19.11270200	2.78656900
H	17.24730700	19.05692700	1.94476600
H	17.84879600	17.61491400	2.78099200
C	17.02688400	20.69305500	4.15420400
H	16.53617900	21.03923600	5.06963100
H	16.46551200	21.08363100	3.29929100
H	18.03783200	21.11879800	4.11995700
C	5.62068500	16.59076200	11.96331300
H	4.65260400	16.69497400	11.48381500
C	15.22846900	9.66361700	7.36155200
H	15.31337400	8.63016200	7.68670100
C	2.90049000	10.68313800	5.81812100
H	2.13625600	10.98565200	5.10793000
C	6.19203100	10.82477200	3.98091200
H	6.51592100	10.11380900	3.21509100
H	5.16789700	11.13718100	3.74720800
H	6.14682500	10.28853300	4.93850500
C	3.56364700	11.64512400	6.57613300
H	3.32388900	12.69799600	6.46158600
C	11.65418800	14.02993100	0.66494600
H	12.48393600	14.29561900	1.31751700
C	11.95161300	9.51228600	2.25233700
H	11.96434800	8.72827000	1.49948900
C	8.68955000	17.24846200	-1.37818700
H	9.15555600	16.26550400	-1.50430900
H	9.45773300	18.01129600	-1.53873300
H	7.92586000	17.37240700	-2.15614900
C	14.23949900	10.49237300	7.89506500
H	13.54421800	10.10337700	8.63535800
C	4.18851300	8.94072500	6.87854300
H	4.41705500	7.88656900	6.99872900
C	12.58102900	10.34174300	4.42127300
H	13.09727300	10.21209500	5.36920400
C	8.11951900	16.27900200	13.16708800
H	9.09257200	16.15653900	13.63264700
C	6.74151100	11.45878000	12.29427200
H	7.59015000	11.80627100	12.87562000
C	12.60248700	9.32406900	3.46850000
H	13.13017100	8.39584900	3.67129500
C	5.88985900	15.46375400	12.72998100
H	5.12587800	14.70070500	12.84334600
C	4.55948400	10.58152900	10.78814000
H	3.70883200	10.24650400	10.20081600
C	9.52943200	13.36849100	-0.99109500
H	8.68989000	13.11368200	-1.63303000
C	3.21178400	9.33510000	5.97020100
H	2.69062800	8.58341000	5.38520700
C	11.72371000	14.31052300	-0.69533600
H	12.60596600	14.79800500	-1.10232500
C	7.13495100	15.30760700	13.33261400
H	7.34143800	14.42322600	13.92888000
C	5.44278200	11.68694500	12.74128600
H	5.27779700	12.20855100	13.67995400
C	10.66163500	13.97130600	-1.53260700
H	10.71164500	14.18847600	-2.59617000
C	4.35391300	11.25165000	11.98827000
H	3.34107000	11.43454800	12.33426800

FCaTHF_anion

Final Single point energy: -4634.992782305024

Ca	4.90867100	8.72929700	12.89557700
F	5.54400100	7.46678500	11.32972300
O	4.67184800	7.85166000	15.08975300
O	4.47749900	10.58635500	11.49360000
N	6.74510100	9.34090400	14.36179400
N	2.66701400	8.12966000	13.40625400
C	7.79088300	10.23126300	14.06013500
C	8.02332400	8.53830000	16.32164500
H	8.88838800	9.10107700	15.99085800
C	0.73194200	9.44837300	12.68483600
C	6.86471600	8.60534700	15.51216200
C	1.57791300	8.32436600	12.54252700
C	7.97675300	11.44396900	14.77536600
C	-0.38408500	9.59377800	11.85991800
H	-1.02049900	10.46907800	11.97952900
C	2.42605400	7.41047600	14.54363100
C	8.08580600	7.76136400	17.47891200
C	0.48348100	10.22359400	15.08468200
C	5.77351000	7.06570300	17.10718400
C	5.76522700	7.81445200	15.94521500
C	1.08142300	10.50888300	13.71950000
H	2.17219500	10.43952900	13.84921200
C	1.19345100	6.81384500	14.89477600

H	0.36489000	6.95203900	14.20998200
C	0.80133200	11.92004400	13.21321100
C	9.01419800	12.30908900	14.42645900
H	9.15880200	13.21774600	15.00771900
C	3.36962900	6.49322800	16.63254900
C	1.34077600	7.44733300	11.45758900
C	9.36236300	7.65633600	18.32595600
C	9.67956100	10.86395800	12.64948500
H	10.34262500	10.63177200	11.81847000
C	9.87264200	12.04668700	13.36080200
C	-0.68456100	8.66763200	10.86251500
C	8.67419300	9.95790800	12.98451200
C	1.02899300	6.07523600	16.06605200
C	1.32000400	12.29505200	11.96640300
H	1.86563600	11.55907200	11.38000100
C	-0.89205300	10.04922200	15.25603000
H	-1.54996700	10.08394500	14.39092400
C	0.21386700	7.62063800	10.65511800
H	0.04530100	6.93261000	9.82830000
C	1.31038200	10.15336500	16.20623400
H	2.38570100	10.25008100	16.07790500
C	-0.31409400	5.43460500	16.44613700
C	3.48787800	7.22454000	15.46684700
C	2.12259800	5.91727600	16.92309000
H	2.01639000	5.32996200	17.82901300
C	2.45233700	6.05714900	9.66777400
C	6.95182500	7.04587600	17.86962900
H	6.97750500	6.44612200	18.77348000
C	7.01849400	11.82515700	15.90205300
H	6.59588600	10.89353100	16.28800200
C	9.01952300	7.45755400	13.06137300
C	0.10435900	12.87676400	13.95153700
H	-0.30054600	12.61745800	14.92532400
C	5.84130900	12.65192900	15.40627300
C	8.53983000	8.63793600	12.23511300
H	7.47249800	8.46072700	12.06072400
C	2.34762400	6.34363300	11.16134100
H	3.32918300	6.74014900	11.45248700
C	1.14657700	13.58203100	11.47323300
H	1.56348900	13.84860500	10.50522600
C	2.13866800	5.09831000	11.99983000
C	-0.07674300	14.16952200	13.45679600
H	-0.62457300	14.89738500	14.04988600
C	4.55452900	6.27215500	17.56567400
C	-1.42838700	9.83492600	16.52209700
H	-2.50092400	9.70184600	16.63851300
C	10.22524500	7.49281800	13.76448100
H	10.81624600	8.40634600	13.76893500
C	5.99367900	13.72943500	14.52858700
H	6.97728300	13.96725300	14.13200800
C	0.77956800	9.93834300	17.47570900
H	1.44195300	9.88084100	18.33562200
C	7.72780400	12.49034900	17.07754800
C	-1.40671000	5.70537100	15.40467000
H	-1.59712800	6.77929800	15.29401400
H	-2.34035200	5.22810000	15.72366900
H	-1.13832200	5.29918900	14.42279800
C	2.17938800	4.81538900	9.09485500
H	1.86632700	3.98756400	9.72421000
C	9.83366500	6.18897600	18.35668100
H	9.07209700	5.53388300	18.79163500
H	10.74699400	6.09718800	18.95768900
H	10.04811600	5.83407500	17.34274800
C	-0.59480800	9.78691400	17.63856200
H	-1.01392500	9.61882900	18.62698500
C	10.67170800	6.37385600	14.46321800
H	11.61709200	6.41344400	14.99835000
C	-0.79382400	6.00007600	17.79683200
H	-0.07696700	5.79052900	18.59748600
H	-1.75493900	5.54912700	18.07423200
H	-0.92534600	7.08520700	17.73306800
C	0.44167200	14.52892400	12.21755900
H	0.30189400	15.53590100	11.83388400
C	4.55683800	12.34130300	15.86167100
H	4.42462000	11.49832100	16.53755000
C	10.51108200	8.50940600	17.77206000
H	10.77721900	8.20913300	16.75299700
H	11.39656400	8.37962700	18.40461900
H	10.26089100	9.57594100	17.76144400
C	-1.92490200	8.80454900	10.01966300
H	-2.75791300	8.23300300	10.44898100
H	-1.76014400	8.42634000	9.00567700
H	-2.24600300	9.84869900	9.95225500
C	0.88912300	4.48347800	12.10333300
H	0.03100800	4.92952900	11.60536300
C	10.95527400	13.01900600	12.97401300
H	10.60096700	13.72201800	12.20891800
H	11.82521800	12.49996600	12.55912300
H	11.28316800	13.61087000	13.83435000
C	4.89352200	14.48578800	14.13221000
H	5.03209800	15.31816700	13.44679700
C	9.07214200	8.11322700	19.76885700
H	8.70472600	9.14503800	19.78585900
H	9.98700600	8.06433000	20.37224800
H	8.31784800	7.47967900	20.24604400
C	2.86878900	7.09846000	8.82705800
H	3.08799100	8.07087400	9.26255600
C	9.16218600	8.68070600	10.84600900
C	3.45271900	13.08660200	15.45566100
H	2.45921000	12.81735500	15.80406300
C	3.61815300	14.16662900	14.59253800
H	2.75385400	14.73877100	14.26575100
C	10.41307700	8.14167200	10.54191700
H	10.98518600	7.63572900	11.31409800
C	-0.14443700	3.90938300	16.58099600
H	0.19270100	3.47465100	15.63453800
H	-1.10007100	3.44555700	16.85612900
H	0.59000000	3.65511100	17.35216200
C	8.25319900	6.29036200	13.09626000
H	7.30518700	6.26774300	12.56121800
C	10.93749200	8.24082200	9.25301700
H	11.91385600	7.81457700	9.03755300
C	0.73348100	3.31094900	12.83643400
H	-0.24516900	2.84274200	12.90534600
C	7.88065800	13.87414500	17.19818700
H	7.45063200	14.53547600	16.45161000
C	9.90107800	5.21374800	14.49430700
H	10.24239500	4.34507500	15.05107900

C	5.51370800	11.88681900	9.76891600
H	6.31839500	11.67192300	9.06043300
H	4.89848700	12.69051100	9.35174400
C	3.00012400	6.90803700	7.45801400
H	3.32867100	7.73038000	6.82758800
C	3.22521400	4.52648800	12.66365900
H	4.19944100	5.00784100	12.59952300
C	4.89819600	11.85525600	12.05422300
H	5.17984500	11.67668800	13.09631400
H	4.06086600	12.56531700	12.02725800
C	8.26398800	11.67478200	18.07918500
H	8.12980400	10.59835100	18.00220100
C	2.30660600	4.62079200	7.71776100
H	2.08686800	3.64478200	7.29272400
C	2.71475500	5.66333800	6.89364800
H	2.81607600	5.51038400	5.82266600
C	1.82499300	2.74531300	13.49362200
H	1.70205800	1.83551500	14.07510600
C	3.07110800	3.36219300	13.41230300
H	3.92555400	2.93631400	13.93197700
C	8.68414300	5.17903400	13.81592500
H	8.06929900	4.28299000	13.84522200
C	6.03922300	12.29173000	11.15581300
H	6.24430300	13.36278300	11.23301800
H	6.95048800	11.73956000	11.41709700
C	8.57298600	14.42422500	18.27564400
H	8.68130300	15.50324800	18.34843100
C	4.90463100	4.76597600	17.57886400
H	5.74759100	4.57002200	18.24993400
H	5.17717700	4.43057400	16.57216000
H	4.04826700	4.17476000	17.92013900
C	8.95612400	12.22039600	19.15592900
H	9.36564800	11.56646100	19.92182500
C	9.11827200	13.60082200	19.25687100
H	9.65517300	14.03061200	20.09806300
C	10.21730500	8.87527700	8.24545900
H	10.62492900	8.94719000	7.24086400
C	4.17375600	6.71598300	18.99614400
H	3.31070000	6.15249600	19.36293700
H	3.92202500	7.78200900	19.00813200
H	5.00345600	6.54872900	19.68953500
C	4.64842000	10.64492600	10.04632200
H	3.65846700	10.71305400	9.57975700
H	5.12258100	9.70483900	9.74585000
C	8.44474000	9.30834700	9.82184900
H	7.46314300	9.71854200	10.04477400
C	8.96150700	9.40829300	8.53548800
H	8.38100700	9.89537200	7.75614200

FCaTHF

Final Single point energy: -5902.592655878604

Ca	4.85171300	8.98783400	13.02274500
P	8.68872900	4.44629300	7.52527500
F	5.47775000	7.69744700	11.46510700
O	4.70801500	7.84488200	15.11622500
O	4.82993400	10.84478500	11.53019600
N	6.79306600	9.29761100	14.37912000
N	2.64755100	8.25082500	13.52419600
C	7.79628300	10.23599700	14.09737800
C	8.10883000	8.41657300	16.27465000
H	8.97163400	8.98131900	15.94029300
C	0.71086300	9.52297000	12.71218900
C	6.93184900	8.52440700	15.49813700
C	1.57302000	8.40519500	12.63283200
C	7.93279100	11.42118700	14.86668300
C	-0.33446800	9.66995500	11.79875800
H	-0.96596000	10.55524900	11.85515000
C	2.42517900	7.50564800	14.64895000
C	8.18623100	7.60258700	17.40522500
C	0.11115200	10.31615300	15.03799800
C	5.85149700	6.95809100	17.07093800
C	5.82685800	7.74371500	15.93400600
C	0.94229300	10.57059700	13.79134100
H	1.99155100	10.45289200	14.09851500
C	1.18426100	6.94826000	15.03121600
H	0.33696900	7.14154300	14.38334400
C	0.81228400	11.98502700	13.23755400
C	8.90447600	12.36250700	14.53455200
H	9.01596300	13.24855400	15.15765200
C	3.41444700	6.48355500	16.66539400
C	1.37917300	7.48921100	11.56828700
C	9.48044900	7.45368500	18.21724800
C	9.57087000	11.06018100	12.64659800
H	10.19842900	10.93409500	11.76821400
C	9.72472600	12.21116100	13.41699700
C	-0.57612200	8.72830400	10.80111500
C	8.64803700	10.06669800	12.97608200
C	1.03487500	6.18317000	16.18752600
C	1.60724800	12.33264400	12.13747500
H	2.27026100	11.58392100	11.71007200
C	-1.28258200	10.22408700	14.98747000
H	-1.79375700	10.30119600	14.03162400
C	0.30659900	7.65330100	10.69344700
H	0.17509400	6.94147200	9.88010000
C	0.74048000	10.18504200	16.27763600
H	1.82666900	10.20575900	16.32834700
C	-0.32327100	5.60825800	16.61747700
C	3.51421900	7.25619600	15.52436400
C	2.15708600	5.94758100	16.98791000
H	2.06329600	5.33562200	17.87872100
C	2.58240100	6.01096400	9.90084500
C	7.05046000	6.89059400	17.79870500
H	7.08955600	6.25807600	18.67936400
C	6.95858700	11.70157100	16.00847100
H	6.59315600	10.73590100	16.36770100
C	9.12981000	7.58078900	12.92090900
C	-0.01569200	12.96197200	13.78894600
H	-0.63167500	12.72582200	14.65158600
C	5.73642900	12.46899500	15.52579500
C	8.53796600	8.77175500	12.17986100
H	7.47272500	8.54295700	12.07493200
C	10.19381500	4.88772500	8.42857900
C	2.37286200	6.35221400	11.37289200
H	3.34056600	6.73676700	11.72426800
C	1.56761700	13.61073200	11.59677700
H	2.19839200	13.85603300	10.74590700
C	2.06828700	5.13587500	12.22527500
C	-0.06196800	14.24762300	13.24496200

H	-0.71716500	14.99269500	13.68892100
C	9.06601900	3.01448800	6.49085100
C	4.62909100	6.17231800	17.53363100
C	-2.02766700	10.03888300	16.14860600
H	-3.11092500	9.97331500	16.08858100
C	10.35319400	7.64896500	13.59035000
H	10.88122700	8.59818900	13.64948400
C	5.84124100	13.61243200	14.72819300
H	6.81792100	13.93668500	14.37855500
C	0.00007300	10.00050600	17.44228800
H	0.51164400	9.89556700	18.39552200
C	7.63959600	12.36225900	17.20276800
C	-1.44326400	5.95711000	15.62940100
H	-1.58228500	7.04114100	15.54551100
H	-2.38638600	5.52199400	15.97903700
H	-1.23666900	5.55713700	14.62990100
C	2.45892800	4.72314300	9.38052500
H	2.16298500	3.90503200	10.03006400
C	9.94088300	5.98330600	18.16944600
H	9.18463700	5.31452000	18.59266400
H	10.86815700	5.85669200	18.74195100
H	10.12757700	5.67450900	17.13457900
C	11.42309600	4.89691200	7.75441300
H	11.48434600	4.62021900	6.70541800
C	-1.38947600	9.93546200	17.38284000
H	-1.97076700	9.79013300	18.28936100
C	10.89156800	6.51791900	14.20058700
H	11.84790100	6.58503100	14.71299600
C	-0.70701000	6.17727900	17.99737600
H	0.02834700	5.90370400	18.76099100
H	-1.68344000	5.78620600	18.31006000
H	-0.76933300	7.26976400	17.95951800
C	7.38030900	4.03228800	8.69072600
C	10.13488200	5.20199800	9.78898200
H	9.19423300	5.18313300	10.32886400
C	0.72467000	14.57776900	12.14709600
H	0.68851700	15.57884500	11.72610000
C	4.46232400	12.05258500	15.92511300
H	4.36192700	11.15827600	16.53876300
C	10.62215100	8.32400100	17.67621900
H	10.86815100	8.06538500	16.64101900
H	11.51876800	8.16530400	18.28599700
H	10.37669100	9.39112200	17.71446500
C	-1.74383200	8.86974400	9.86109400
H	-2.61789100	8.32053000	10.23402800
H	-1.50686800	8.46916800	8.87030200
H	-2.03926600	9.91764600	9.75046900
C	0.81594600	4.51819200	12.19628100
H	0.02125700	4.94770400	11.59022700
C	10.72480700	13.27332700	13.04365100
H	10.23287800	14.12968300	12.56484100
H	11.47090300	12.88687700	12.34292000
H	11.24713900	13.65553000	13.92724800
C	4.70932200	14.33371000	14.35876800
H	4.81483600	15.21966700	13.73758000
C	9.22848900	7.85159100	19.68440300
H	8.88243500	8.88921400	19.75247900
H	10.15520900	7.75972400	20.26403200
H	8.47285800	7.21245400	20.15167900
C	2.98343900	7.03683600	9.03414400
H	3.07867200	8.04692300	9.42334500
C	9.06778700	6.56915400	5.76769500
H	10.13206600	6.41942600	5.91946500
C	9.07670200	8.84132200	10.75884800
C	3.32820600	12.77114400	15.55341400
H	2.34411000	12.43602600	15.86771000
C	3.44733000	13.91676200	14.77194400
H	2.55841400	14.46403200	14.47120900
C	11.30033100	5.53560800	10.46966500
H	11.24503400	5.78352500	11.52572200
C	8.12959000	5.79721900	6.45991700
C	10.44252600	8.85043100	10.46023300
H	11.17204900	8.78789400	11.26311800
C	-0.23889500	4.07386000	16.72303300
H	0.02349600	3.63567200	15.75498300
H	-1.20630100	3.66344400	17.03855500
H	0.51514700	3.76161600	17.45288800
C	8.44062600	6.36512800	12.90173600
H	7.47052700	6.31833400	12.40973000
C	8.49632400	2.89934400	5.21989600
H	7.86190900	3.68824600	4.82630700
C	9.88745000	1.99973800	6.99664600
H	10.33107700	2.09018100	7.98450800
C	12.51934500	5.55580000	9.80010600
H	13.42766100	5.81690200	10.33581100
C	10.88464400	8.92626700	9.14269900
H	11.95116500	8.93825600	8.93331200
C	6.98349400	2.70252000	8.85737900
H	7.41834400	1.91420900	8.25075400
C	0.57969600	3.35702000	12.92569300
H	-0.39931600	2.88597600	12.88971900
C	7.63327800	13.73837000	17.43894400
H	7.08956300	14.40205700	16.77313100
C	10.20194600	5.30768500	14.16961400
H	10.61826000	4.42856300	14.65405800
C	5.48214600	11.63027400	9.36194100
H	5.97962400	11.18771100	8.49428500
H	4.86804800	12.46895300	9.01729400
C	3.25326400	6.78447900	7.69619900
H	3.56060800	7.60056700	7.04722600
C	10.13425300	0.87143500	6.22433600
H	10.77176200	0.08334600	6.61331300
C	3.06833600	4.58365200	13.02657200
H	4.03724700	5.07654700	13.08227600
C	5.62122000	12.05166500	11.68743500
H	6.19164600	11.95309500	12.61602000
H	4.94723000	12.91682900	11.76557200
C	8.32366400	11.53742000	18.10283700
H	8.31218900	10.46292300	17.93480300
C	12.57998500	5.23701800	8.44454700
H	13.53219100	5.24198800	7.92265200
C	2.72618500	4.46435500	8.03461100
H	2.62353800	3.45129400	7.65408600
C	3.12514600	5.49064400	7.18620200
H	3.33017200	5.28989800	6.13762000
C	8.75244000	1.76597200	4.45537300
H	8.31529600	1.67656100	3.46560500
C	6.80435900	5.04891500	9.46593000

H	7.10260100	6.08760500	9.33816600
C	9.56883300	0.75504200	4.95580900
H	9.76832000	-0.12688100	4.35398400
C	1.59267500	2.80081900	13.70591200
H	1.40796000	1.89566900	14.27804100
C	8.63310400	7.55110200	4.88644000
H	9.36209500	8.15404300	4.35343100
C	2.83625400	3.42437800	13.76302500
H	3.62659100	3.01026800	14.38399900
C	8.96794700	5.23726900	13.52454800
H	8.41251800	4.30262300	13.50956000
C	6.47200000	12.10461000	10.43349200
H	6.86365900	13.10673000	10.23761200
H	7.31248700	11.40763100	10.52819000
C	7.26996700	7.76641500	4.69624100
H	6.93390200	8.53774300	4.00925900
C	8.31292800	14.27635400	18.53197400
H	8.29581700	15.35051100	18.69701800
C	4.93592300	4.65980600	17.43635800
H	5.79260000	4.39719300	18.06636000
H	5.17042200	4.38644700	16.40160200
H	4.07245900	4.07009300	17.76238600
C	5.45764800	3.39896800	10.59104800
H	4.70412200	3.15231700	11.33403700
C	6.76025800	6.00842300	6.26876000
H	6.02560500	5.41066700	6.80015000
C	9.00326300	12.07019200	19.19250800
H	9.52816000	11.40843400	19.87712800
C	5.84777500	4.72610600	10.41889900
H	5.42027800	5.53225300	11.00953400
C	6.33730900	6.99697300	5.38631200
H	5.27488600	7.16323200	5.23780400
C	6.01821300	2.39283800	9.81032300
H	5.70521000	1.36106200	9.93922100
C	9.00452700	13.44754400	19.41024600
H	9.53112800	13.86838200	20.26239100
C	9.96771600	8.97022400	8.09507600
H	10.31413400	9.02193400	7.06675500
C	4.31923300	6.53379100	19.00309800
H	3.46181300	5.96432400	19.37313400
H	4.09050500	7.60139300	19.09135400
H	5.17299300	6.30903600	19.64910300
C	4.61882200	10.60206800	10.10262500
H	3.54975700	10.70975500	9.88311500
H	4.92573600	9.56838400	9.91280700
C	8.16599100	8.86869000	9.69720900
H	7.10240200	8.81996200	9.92159200
C	8.60410200	8.92919600	8.37641700
H	7.87908700	8.93416500	7.56564800

F_anion

Final Single point energy: -99.957248904643

F	16.07104000	0.83903000	12.51927000

Fpentane

Final Single point energy: -296.937128361209

C	-1.97903100	-2.05591900	-0.00406800
H	-1.63804600	-3.09716700	-0.03678000
H	-1.63691100	-1.56423600	-0.92210300
H	-3.07396700	-2.06071300	-0.01384200
C	-1.43545600	-1.34244000	1.23222400
H	-1.80894100	-0.30978200	1.25854100
H	-1.81393700	-1.83251700	2.13958100
C	0.09259700	-1.32376600	1.27300300
H	0.47284900	-0.83285400	0.36562200
H	0.46789100	-2.35689000	1.24957000
C	0.63964200	-0.60804900	2.51017900
H	0.27563100	-1.10414100	3.41948300
H	0.27739900	0.42809700	2.53227700
C	2.15037200	-0.60512900	2.51812000
H	2.56006500	-0.07200600	1.65172200
H	2.55837500	-1.62270600	2.54586000
F	2.62608700	0.06145500	3.67534200

K_cation

Final Single point energy: -599.929363225165

K	16.07104000	0.83903000	12.51927000

NaxF3

Final Single point energy: -4402.570263971476

Ca	10.89911200	15.42741000	6.04779800
O	11.39140800	17.22375700	4.54961700
F	10.03036100	14.95633500	7.88813300
N	13.18337500	15.95919300	6.09285600
N	9.54443000	15.34236000	4.13760200
C	14.01797700	15.57884900	7.15462200
C	15.00419100	17.28694900	5.06401700
H	15.73209100	16.76709200	5.67673100
C	12.73063100	17.60124200	4.40392800
C	10.59861400	17.35837700	3.40184400
C	8.75658500	14.22231900	3.82701900
C	13.64868500	16.92067000	5.22988300
C	15.40905300	18.24590700	4.13657200
C	14.22101500	16.43737900	8.26589900
C	14.43733200	18.91058500	3.37298200
H	14.73802900	19.66839600	2.65962900
C	10.83623500	18.38342500	2.50525300
C	7.43039700	14.09757800	4.29941200
C	14.35005000	18.98376300	7.94295400
C	13.07877600	18.60446300	3.51688500
C	15.71528600	19.07357300	8.21604900
H	16.23231800	18.22764500	8.66042000
C	9.63206500	16.34824300	3.21301000
C	8.84071700	16.47306700	2.04687600
H	8.08898300	15.71053400	1.87677600
C	9.02472300	17.50724100	1.13016200
C	12.82853100	17.96162300	9.68362700
C	13.71458600	20.07911200	7.34897200
H	12.65205300	20.01657900	7.12135800
C	6.69818700	12.94150800	4.02470600
H	5.68537500	12.85371300	4.41481100
C	6.04738600	16.23734500	4.28728900
C	4.61498300	14.62714100	6.28262000
H	4.06261500	15.00257400	5.42520400
C	13.50710700	17.77937200	8.32776900
H	12.70044800	17.72574600	7.58441000
C	14.57877600	14.28122100	7.20887100
C	15.78238500	21.32140700	7.32992900

H	16.33863500	22.22348200	7.08966400
C	14.31060100	11.86333500	6.52855600
C	15.25330400	13.55154700	4.88140500
C	6.00930600	14.69103800	6.29044500
C	7.23186900	11.89049800	3.28091800
C	14.32805400	13.31284900	6.06246900
H	13.31635600	13.52438700	5.68665100
C	14.42149800	21.23629400	7.03939200
H	13.91033200	22.07218500	6.56875700
C	15.61444700	14.76280100	9.36297200
C	6.82201700	15.22615900	5.11758700
H	7.67009700	15.77483000	5.54720600
C	16.42563100	20.23437400	7.91535700
H	17.48944500	20.28495100	8.13325600
C	15.00507900	16.01637000	9.33921100
H	15.11709100	16.67535900	10.19924200
C	10.03129600	18.45718400	1.36217700
H	10.18641000	19.26188300	0.65389200
C	6.69775600	14.21793200	7.41429200
H	7.78531900	14.27870300	7.44163500
C	15.36692600	13.90161600	8.29488800
H	15.78844800	12.89818600	8.31424900
C	10.79198300	13.18634500	2.72645900
H	11.27939800	13.83043900	3.47472300
C	9.32597900	13.12646300	3.13032000
C	11.94526700	19.37740800	2.84250200
C	8.55814400	11.99545200	2.86013000
H	9.01686200	11.15854800	2.33570300
C	13.27913100	18.86592400	10.64572100
H	14.13520200	19.49987800	10.43093000
C	11.71681100	17.16325800	9.98093800
H	11.34957000	16.45036000	9.24302600
C	16.89227800	18.55455300	3.89099800
C	15.25532400	10.92109000	6.12574800
H	16.04659700	11.21066500	5.44000300
C	17.80788800	17.88902000	4.92637500
H	17.73648500	16.79710000	4.88752000
H	17.56436700	18.21618800	5.94367500
H	18.84872700	18.16332800	4.72005300
C	16.59643800	13.89325900	5.04783800
H	16.99338300	14.03574300	6.05002900
C	14.75840300	13.38978600	3.58581500
H	13.71514500	13.11690600	3.44597500
C	11.03380600	13.87461000	1.39570100
C	8.12366700	17.66189000	-0.10305600
C	12.63988100	18.96590700	11.88228300
H	13.00732200	19.67417500	12.62043500
C	11.48328200	11.83019700	2.82332600
C	6.07142900	17.58186300	4.67028200
H	6.68110500	17.88050400	5.52086300
C	5.27124200	15.87121300	3.18635700
H	5.25583700	14.83444300	2.86043700
C	10.29179500	13.55135000	0.25834500
H	9.47984700	12.83181800	0.33492600
C	3.92196700	14.08912600	7.36713200
H	2.83615200	14.04564300	7.34240200
C	11.53653600	18.16858300	12.16960700
H	11.03592000	18.25024000	13.13060900
C	13.29517300	11.45979400	7.40470400
H	12.55146000	12.18687300	7.72708400
C	16.49909500	14.34915800	10.50871100
H	16.19131900	14.83302200	11.44109500
H	17.54324300	14.63255700	10.32324300
H	16.47652800	13.26498000	10.65655900
C	11.07498200	17.26682200	11.20972000
H	10.21008400	16.64232900	11.41857400
C	4.61395400	13.61538000	8.47784700
H	4.07368800	13.20130700	9.32489100
C	12.11453200	11.21434800	1.74230500
H	12.09738300	11.68824000	0.76548800
C	17.42706200	14.06027000	3.94170100
H	18.47129100	14.32460200	4.08740400
C	15.19188300	9.60604700	6.58993100
H	15.93727700	8.88568500	6.26291600
C	6.00712400	13.68597600	8.49807100
H	6.55840100	13.32990400	9.36466800
C	4.52213200	16.82241900	2.49655000
H	3.92258100	16.51856500	1.64226300
C	4.54895000	18.15792500	2.88902700
H	3.97238200	18.90085700	2.34453200
C	11.39245700	20.39542100	3.87243200
H	12.18183200	21.09703900	4.16719300
H	11.03091200	19.88540000	4.77097400
H	10.56071200	20.95914000	3.43406300
C	7.21362200	16.44592700	-0.31841600
H	6.52402500	16.30219800	0.51969600
H	7.79866500	15.52776600	-0.44753200
H	6.61339900	16.59739400	-1.22285600
C	11.54095000	11.20091900	4.07369400
H	11.06170200	11.67163900	4.93062900
C	15.58051000	13.57001000	2.47740500
H	15.16944900	13.45219800	1.47763100
C	5.33355900	18.53656300	3.97710800
H	5.37330800	19.57828900	4.28453700
C	16.92224300	13.90347300	2.65263400
H	17.56846500	14.04679600	1.79083800
C	12.42372700	20.14646100	1.61033600
H	11.60005700	20.71779200	1.17284100
H	12.82663000	19.47296100	0.84611600
H	13.19947000	20.86620300	1.88734000
C	7.23465500	18.90624400	0.09092300
H	6.56524300	19.03604100	-0.76905400
H	7.84211900	19.81191200	0.19324400
H	6.62145300	18.80196500	0.99325900
C	17.27745800	18.02744700	2.49432000
H	18.33775300	18.22381300	2.29062900
H	16.68191500	18.51083200	1.71245800
H	17.10793000	16.94599900	2.43296100
C	17.14623400	20.07243600	3.94315700
H	16.85929100	20.47642200	4.92000000
H	16.58388700	20.60923300	3.17314600
H	18.21159600	20.27861600	3.78292900
C	14.18150100	9.21616100	7.46201400
H	14.13046500	8.19179600	7.82094800
C	6.40836400	10.67417000	2.95064100
H	5.93659100	10.77465000	1.96471500
H	5.60873400	10.52630900	3.68284600
H	7.02671200	9.77124700	2.92429800

C	12.06059300	14.81400900	1.28456600
H	12.63083300	15.09113500	2.16933200
C	12.78286700	9.99942600	1.90445000
H	13.27043100	9.53865100	1.04922000
C	8.97097000	17.84542200	-1.37584300
H	9.62374800	16.97991200	-1.53133500
H	9.59805200	18.74077400	-1.32666400
H	8.31448900	17.94509100	-2.24889000
C	13.22847000	10.15226000	7.86806500
H	12.42925900	9.85883800	8.54377900
C	12.21003200	9.99586900	4.23987000
H	12.26389400	9.54168700	5.22539000
C	12.83509200	9.38642200	3.15137200
H	13.36506000	8.44662600	3.28103600
C	10.58324200	14.14079200	-0.96885800
H	9.99718700	13.87893000	-1.84610800
C	12.35119000	15.41100900	0.06099200
H	13.14770500	16.14811100	-0.00330000
C	11.61751900	15.06938300	-1.07293400
H	11.84202300	15.53294800	-2.02978700

PPh4_cation

Final Single point energy: -1267.566210113942

P	6.10765700	2.62681100	11.36371900
C	5.19082200	2.05568300	9.91657700
C	6.84604700	4.22265900	10.95243300
C	5.00107500	2.79640700	12.78072900
C	3.61743200	2.87278900	12.60142100
H	3.18092800	2.79407400	11.61051900
C	4.40141500	2.97598200	9.21447500
H	4.36862000	4.01980000	9.51577500
C	5.55747400	2.87690800	14.06398400
H	6.63252500	2.80381500	14.20584800
C	7.44534300	4.38645700	9.69674100
H	7.43622100	3.57869500	8.96963900
C	6.84419700	5.26823600	11.87944500
H	6.36761900	5.15002400	12.84768800
C	7.02376800	0.26926400	12.48755300
H	5.98920100	0.09878700	12.77388500
C	8.05053500	5.59633300	9.38071200
H	8.51594200	5.72561200	8.40842300
C	7.45023900	6.47603400	11.54917700
H	7.44483000	7.29155700	12.26578500
C	8.05345600	6.63926000	10.30527300
H	8.52335100	7.58511000	10.05171600
C	7.39200900	1.43678500	11.80618700
C	8.72542400	1.66112100	11.45342300
H	9.01838700	2.57138800	10.93953000
C	3.71124500	1.21259800	7.72183900
H	3.13540000	0.88305400	6.86190100
C	5.24538100	0.71786100	9.51711000
H	5.86783900	0.00463900	10.04848200
C	2.79271300	3.03703200	13.70963400
H	1.71694800	3.09027800	13.57332000
C	3.66123900	2.54719700	8.11995600
H	3.04903500	3.25877200	7.57437600
C	4.72322900	3.04449100	15.16207200
H	5.15223600	3.10653300	16.15743400
C	7.99394100	-0.67378000	12.80256000
H	7.71057400	-1.57916700	13.33045800
C	4.50243400	0.30212900	8.41696100
H	4.54848600	-0.73545000	8.10085300
C	3.34317800	3.12480800	14.98531700
H	2.69421600	3.24997600	15.84722500
C	9.68792800	0.71071300	11.77810600
H	10.72539100	0.88603000	11.51051800
C	9.32376700	-0.45388500	12.44826500
H	10.07969400	-1.19152000	12.70165500

THFCa_addBr

Final Single point energy: -7109.286784417035

Ca	0.06719000	3.47762200	4.03939600
Br	1.68189300	0.38095500	7.38169200
O	-0.35161700	5.75319400	3.90796600
O	-0.37581300	3.68523600	1.73569100
N	-1.94376400	4.10009800	5.14031000
N	2.06171900	4.71084600	3.82261500
C	-2.50236000	5.26225700	4.66595900
C	-1.66696700	6.17979800	3.98238400
C	3.02881700	7.46819100	6.02479900
C	1.88011400	5.94931000	3.24255000
C	-4.54284500	1.67741300	7.46516200
C	-2.79078800	3.36769000	7.32568700
C	-2.10136700	7.36290100	3.42164800
C	3.70863600	5.04937100	5.59944300
C	2.75404300	5.99917600	6.30582200
H	1.75485700	5.79019800	5.89685700
C	-2.79972300	3.28796400	5.91615500
C	2.89686500	6.73200900	2.66326300
H	3.90849200	6.34564400	2.71613300
C	-3.66877600	2.57786600	8.06937900
H	-3.65904000	2.65758900	9.15442200
C	-3.86020200	5.63358900	4.76744400
H	-4.52158500	4.96275800	5.30265900
C	-4.34711600	6.82209200	4.21942900
C	2.63066500	7.95537500	2.04388700
C	0.57963200	6.50831300	3.21558900
C	2.67051800	5.70233800	7.80221300
C	-2.25979000	5.75472000	7.96092800
C	0.26744400	7.72115100	2.63361700
C	4.25647000	3.57280200	3.75134300
C	3.34081800	4.45779200	4.36039400
C	4.32202900	7.98060700	5.90704100
H	5.17337400	7.30678100	5.94403600
C	4.94209700	3.34799400	1.34682300
C	4.92918600	4.73648400	6.18797600
H	5.17161800	5.16987500	7.15746000
C	1.95247400	8.35609400	5.95062500
H	0.93946600	7.96543600	6.01680100
C	-3.46492500	7.67445000	3.54785500
H	-3.83240600	8.59655200	3.10984700
C	-5.83152500	7.19981200	4.31320800
C	1.31442200	8.42803000	2.02110300
H	1.08998500	9.37490900	1.54150100
C	-1.14073100	8.31140200	2.70762600
C	-4.50214400	1.55758300	6.07632800
H	-5.16008100	0.84297900	5.58747200
C	2.85911700	6.67366600	8.78592800

H	3.09121900	7.69523200	8.49957800
C	-3.64672900	2.33866800	5.30293900
C	2.46330400	5.04384500	10.52793300
H	2.38200600	4.78763200	11.58094100
C	-1.80952000	4.30750600	8.01495000
H	-0.88007900	4.25609200	7.42809100
C	2.36849200	4.39531100	8.20505500
H	2.21790100	3.62026000	7.45527400
C	3.74734300	1.41676300	2.47455800
C	-3.57221500	6.12082600	8.26553400
H	-4.29707100	5.35034800	8.51877300
C	-1.45336900	3.84298000	9.42303100
C	5.47821500	3.29440600	4.37102000
H	6.16805900	2.60371200	3.89115300
C	2.75347500	6.34704100	10.13953000
H	2.90348200	7.11935500	10.88965400
C	-1.34439300	6.75379800	7.62919800
H	-0.31939400	6.47346400	7.39261700
C	6.15196000	2.66813900	1.16671200
H	6.36776900	1.78434100	1.76120200
C	3.93369900	2.92975600	2.41073400
H	2.96955500	3.35944600	2.11351600
C	-5.46444400	0.82010000	8.29134200
H	-4.96174200	-0.10206300	8.60967400
H	-6.35274600	0.52971700	7.72212400
H	-5.78675900	1.34375100	9.19666400
C	-1.66254500	4.61995400	10.56200300
H	-2.10459000	5.60768300	10.46989700
C	2.15848900	9.72080900	5.77521600
H	1.30597700	10.39237400	5.71442100
C	5.83658300	3.86101000	5.58818700
C	-0.86702600	2.58059800	9.57594600
H	-0.67297700	1.96937700	8.69678300
C	-6.44113100	7.20425100	2.89771700
H	-7.50532300	7.46725500	2.94139600
H	-6.34988500	6.21364400	2.43604600
H	-5.93618700	7.92836100	2.24987000
C	-0.51265600	2.10296000	10.83041600
H	-0.05057200	1.12298700	10.92015700
C	-3.55592700	2.15532000	3.79661100
H	-3.39420700	3.15892700	3.37619800
C	3.66131300	10.24328800	1.72357800
H	3.75861900	10.36807400	2.80773200
H	2.71860500	10.70117300	1.40943400
H	4.47575200	10.79371200	1.23759500
C	2.27206300	4.06647000	9.55064200
H	2.03479900	3.04588000	9.83511700
C	-1.65684400	8.59278800	1.28011600
H	-2.64119400	9.07022400	1.30925300
H	-1.74279100	7.66073200	0.71136200
H	-0.97440100	9.26205000	0.74708300
C	3.73741000	8.75359900	1.34225900
C	3.45378200	10.22305400	5.66681100
H	3.61886400	11.28771500	5.52505800
C	4.53359700	9.34590200	5.72734800
H	5.54803500	9.72448700	5.63113100
C	-3.04373400	8.44698000	7.89146400
H	-3.34999600	9.48904200	7.85583600
C	7.07457200	3.09296000	0.21579500
H	8.00876900	2.55102200	0.09393000
C	4.67547700	4.45247500	0.53409000
H	3.73862900	4.99113500	0.65802400
C	-1.30462100	4.14351400	11.82498900
H	-1.47446500	4.76606800	12.69970700
C	-0.73312900	2.88366100	11.96584900
H	-0.45395700	2.51392800	12.94886300
C	-5.97855500	8.60349300	4.93143800
H	-5.48467500	9.36876300	4.32480400
H	-5.53741100	8.62833000	5.93412000
H	-7.03937100	8.87010400	5.01278600
C	-1.73164200	8.09075600	7.58682600
H	-1.00871900	8.85660600	7.31618800
C	-3.96091300	7.45691000	8.23959500
H	-4.98672200	7.72524600	8.47877600
C	3.59815500	0.73480400	3.68350700
H	3.62441800	1.28309600	4.62107200
C	-1.08842000	9.64023700	3.49572400
H	-0.40769200	10.35094800	3.01565900
H	-0.73732000	9.45928700	4.51699000
H	-2.08331300	10.09460600	3.54667900
C	0.64568300	3.44926200	0.72122600
H	1.06845700	2.45344700	0.89297900
H	1.42395500	4.21421400	0.84088100
C	6.80094500	4.20175600	-0.58372300
H	7.51899900	4.52965100	-1.33028900
C	5.13959600	8.24852500	1.70921800
H	5.30843500	7.22200700	1.36711500
H	5.30312800	8.28380400	2.79271300
H	5.89203200	8.88438700	1.22927300
C	7.14026300	3.52340300	6.26093600
H	6.97487000	2.89610700	7.14559800
H	7.65816400	4.42749000	6.59951500
H	7.80542100	2.97879800	5.58458200
C	5.59447300	4.87709900	-0.42376900
H	5.36454000	5.73684300	-1.04792100
C	3.54906800	8.61260500	-0.18112600
H	4.33862200	9.15295100	-0.71839800
H	2.58017200	9.01613200	-0.49509300
H	3.59056000	7.55753500	-0.47597900
C	-4.84658400	1.64649900	3.18670300
C	-2.32545500	1.34817800	3.38443200
C	-6.63344900	6.21904000	5.17842500
H	-7.67756600	6.54773100	5.22606300
H	-6.24383800	6.17668500	6.20207600
H	-6.62131700	5.20491500	4.76333200
C	-7.04014300	2.14837400	2.28101700
H	-7.78308400	2.88247100	1.98039500
C	3.42810000	-0.64978500	3.70857000
H	3.31531000	-1.15373800	4.66491500
C	3.68286000	0.67717800	1.28517000
H	3.78245800	1.18974000	0.33133300
C	-1.53702400	4.31779400	1.11278200
H	-1.84140100	5.16746400	1.73155100
H	-2.34827900	3.57985300	1.08077700
C	3.40217200	-1.37689200	2.52333800
H	3.27947400	-2.45638600	2.54336700
C	-1.33229500	0.97208200	4.29816200
H	-1.48002900	1.14761200	5.36229600

C	-1.07881800	4.70645700	-0.28407400
H	-1.91405700	4.75564500	-0.98768500
H	-0.57559200	5.68057700	-0.26363100
C	3.51974600	-0.70325100	1.30709100
H	3.48383200	-1.25613400	0.37184000
C	-5.11959600	0.28421500	3.04210400
H	-4.37092600	-0.44815800	3.33514400
C	-5.81874500	2.57149900	2.79737400
H	-5.61040500	3.63479700	2.90487500
C	-7.30561400	0.78707100	2.14429800
H	-8.25663800	0.45289400	1.73885900
C	-6.34067500	-0.14283800	2.52584100
H	-6.53871500	-1.20631700	2.42162700
C	-0.14752200	0.36691400	3.86503300
H	0.60847900	0.09346300	4.59948400
C	-0.07203200	3.59965600	-0.60798400
H	-0.59090200	2.67102100	-0.87332000
H	0.61727800	3.86371100	-1.41444200
C	-2.13033000	1.03298600	2.03416100
H	-2.90342800	1.28466800	1.31234900
C	0.04851500	0.10526900	2.51064200
H	0.97261900	-0.35454900	2.17416300
C	-0.95980100	0.42092100	1.60168000
H	-0.82591000	0.20298000	0.54530400

THFCaBr_anion

Final Single point energy: -7109.311977811371

Ca	0.30161200	3.53700700	4.45673500
Br	1.27221300	1.74667800	6.42826700
O	-0.30593400	5.75580500	3.87163200
O	0.02091900	3.07197200	2.12893400
N	-1.92334800	4.05889600	5.03857100
N	2.15337200	4.97934700	4.17141800
C	-2.48863700	5.18555700	4.49871500
C	-1.64353100	6.11634200	3.84112700
C	3.43635200	7.51355600	6.34312900
C	1.97291900	6.16774000	3.52555600
C	-4.50439100	1.63247100	7.37824000
C	-2.78159100	3.34578400	7.21332200
C	-2.09004700	7.28035600	3.24854700
C	3.93494700	5.06089500	5.84853300
C	3.11273600	6.05909700	6.65102200
H	2.07266200	5.90382500	6.33628600
C	-2.77670300	3.23743100	5.79986800
C	2.98836100	6.99239700	2.99620400
H	4.01256700	6.66024200	3.12479100
C	-3.64871200	2.56177800	7.97000700
H	-3.64533900	2.66247900	9.05336300
C	-3.85793900	5.52671700	4.54320000
H	-4.52226800	4.84984400	5.06704500
C	-4.35353600	6.69303100	3.95673000
C	2.69814500	8.17609400	2.31590500
C	0.64180900	6.61914900	3.34010900
C	3.15533300	5.79884600	8.15214600
C	-2.26400000	5.75583100	7.75848300
C	0.31104100	7.79639800	2.70018600
C	4.21049600	3.68550000	3.86241400
C	3.43952700	4.61450100	4.59513200
C	4.73250700	7.95350200	6.07290300
H	5.54041800	7.22945800	6.00271200
C	4.30270700	4.05941300	1.35736000
C	5.14167700	4.56404600	6.33211700
H	5.49646600	4.89175400	7.30810500
C	2.40826700	8.45887400	6.40244000
H	1.39158400	8.12477000	6.59796000
C	-3.46675300	7.55300000	3.30459600
H	-3.83917000	8.45657100	2.83318900
C	-5.84536300	7.04982900	3.99857200
C	1.36207700	8.57020800	2.18185100
H	1.12197800	9.48805500	1.65510000
C	-1.13742400	8.25235500	2.55762000
C	-4.43729200	1.47354200	5.99735200
H	-5.06361800	0.71966300	5.52755900
C	4.07513700	6.42221600	8.99985800
H	4.78373400	7.13831400	8.59205000
C	-3.59135400	2.24971000	5.20377000
C	3.16942400	5.24936000	10.90847300
H	3.17106700	5.04078600	11.97505700
C	-1.81146200	4.31393700	7.88200400
H	-0.87593900	4.24006800	7.30817700
C	2.23844500	4.90187100	8.70890700
H	1.51773300	4.40470900	8.06309000
C	3.87643800	1.73301200	2.27297200
C	-3.56254400	6.13702300	8.10340100
H	-4.26817300	5.38110400	8.44106800
C	-1.46655300	3.91094400	9.31189600
C	5.41053700	3.20083000	4.38691600
H	5.97006400	2.45415100	3.82497100
C	4.08743000	6.14489100	10.36546500
H	4.81238500	6.63896200	11.00725600
C	-1.37390700	6.73237300	7.31289800
H	-0.36509100	6.44086600	7.02568200
C	5.65766300	4.38792900	1.28103900
H	6.32904000	4.09701900	2.08418800
C	3.72506300	3.23384200	2.49527400
H	2.64497600	3.43999300	2.48362600
C	-5.46465100	0.82581100	8.21134100
H	-5.01506800	0.53622700	9.16678700
H	-5.77850000	-0.08143900	7.68653600
H	-6.36862600	1.40446800	8.44037300
C	-1.66160200	4.74680900	10.41140400
H	-2.08118100	5.73808700	10.26872800
C	2.66711700	9.81135900	6.20891500
H	1.85200800	10.52938200	6.25099600
C	5.89733400	3.63028100	5.61814200
C	-0.90524300	2.64541800	9.53095100
H	-0.72812300	1.99227700	8.67998300
C	-6.39293300	7.11491200	2.55958700
H	-7.46681500	7.33924800	2.56988400
H	-6.24603300	6.15679000	2.04858600
H	-5.88872800	7.89044400	1.97388900
C	-0.57071700	2.22165200	10.81074500
H	-0.13431100	1.23652400	10.95451400
C	-3.48721000	1.96822300	3.70646500
H	-2.96447700	2.83104600	3.27049500
C	3.70273400	10.48588700	2.17227900
H	3.83096900	10.52644700	3.25901500
H	2.73679000	10.93807400	1.92612100

H	4.48811600	11.09518100	1.70802500
C	2.24182900	4.62941000	10.07347600
H	1.51044000	3.93806000	10.48311800
C	-1.50060200	8.33629700	1.05809700
H	-2.53209300	8.68067000	0.92865400
H	-1.40386800	7.35164900	0.58691900
H	-0.83749300	9.03536100	0.53798300
C	3.79580800	9.03304300	1.66989000
C	3.96943700	10.24368900	5.96171000
H	4.17712600	11.30004000	5.81409400
C	4.99875900	9.30893900	5.88959200
H	6.01521100	9.63448800	5.68330000
C	-3.06592500	8.43578600	7.55796000
H	-3.37968100	9.47259000	7.47072600
C	6.15753000	5.08978800	0.18641300
H	7.21484100	5.33849300	0.14452200
C	3.45945500	4.46511300	0.32063500
H	2.39909800	4.23034000	0.38168600
C	-1.32300400	4.32492400	11.69876200
H	-1.48396400	4.99360500	12.54039600
C	-0.78309700	3.06072200	11.90593800
H	-0.52047100	2.73236600	12.90796800
C	-6.03296500	8.42406300	4.67009500
H	-5.50323400	9.21340200	4.12742800
H	-5.65120600	8.40436800	5.69697100
H	-7.09733700	8.68820900	4.70119500
C	-1.76992100	8.06341500	7.20844800
H	-1.06828400	8.80950100	6.84382900
C	-3.96015400	7.46739300	8.01178600
H	-4.97446400	7.74790800	8.28375100
C	3.28505600	0.86242800	3.19729800
H	2.78935400	1.26886000	4.07774100
C	-1.28760200	9.65194200	3.19545000
H	-0.62366400	10.37326300	2.70897400
H	-1.03409300	9.61109000	4.26047900
H	-2.31481700	10.01625200	3.09787400
C	0.28420000	1.87190100	1.34358900
H	0.06706900	1.00701500	1.97660000
H	1.34575600	1.86181300	1.06017400
C	5.30886500	5.48032800	-0.84689500
H	5.69907900	6.03401300	-1.69662300
C	5.20356400	8.50987600	1.97953200
H	5.35570400	7.50019500	1.58221000
H	5.39596800	8.48965400	3.05818100
H	5.94678000	9.16752600	1.51420400
C	7.17614100	3.07779000	6.18987500
H	6.96962300	2.34867400	6.98339900
H	7.78923300	3.87057600	6.63178700
H	7.76734900	2.57291100	5.42028600
C	3.95296400	5.16866300	-0.77392700
H	3.27691100	5.48009200	-1.56601000
C	3.60515400	9.02076600	0.14023300
H	4.39315000	9.61017100	-0.34553700
H	2.63674100	9.44619200	-0.14304000
H	3.65538000	7.99560100	-0.24334800
C	-4.85241900	1.89788300	3.04363000
C	-2.59732700	0.75488300	3.42499900
C	-6.67359700	6.02336800	4.78154800
H	-7.72572300	6.32993000	4.78164700
H	-6.34339800	5.95185900	5.82432700
H	-6.61463300	5.02546600	4.33230800
C	-6.65293400	3.02748300	1.86886800
H	-7.04716600	3.92894600	1.40722900
C	3.32452900	-0.51358700	3.01345100
H	2.85173300	-1.16655600	3.74304800
C	4.51904700	1.18403400	1.16278000
H	4.98225600	1.83638700	0.42813200
C	-0.58565700	4.09128200	1.26763600
H	0.00157400	5.01133200	1.35424300
H	-1.60279200	4.27530900	1.63693200
C	3.96885700	-1.05388100	1.89944100
H	4.00344600	-2.13004700	1.75329500
C	-1.60558300	0.36878800	4.33284900
H	-1.50674400	0.89274900	5.27989100
C	-0.58012100	3.50415100	-0.13876900
H	-1.43322400	3.85631100	-0.72481400
H	0.33970300	3.77818700	-0.66751100
C	4.56760300	-0.19947600	0.97981500
H	5.07518500	-0.60639800	0.10900900
C	-5.62188600	0.72835800	3.03689700
H	-5.21810200	-0.18495900	3.46599300
C	-5.38440900	3.04318800	2.44538600
H	-4.79868000	3.96039900	2.44531200
C	-7.41339400	1.86159800	1.87954700
H	-8.40199800	1.84685800	1.42896100
C	-6.89015500	0.70997100	2.46481400
H	-7.46967800	-0.20947400	2.47208100
C	-0.74565600	-0.69203100	4.05399200
H	0.02066100	-0.95755100	4.77717200
C	-0.61312600	1.99672100	0.12542200
H	-1.62938400	1.67001100	0.36833500
H	-0.24451300	1.40403400	-0.71647400
C	-2.69527900	0.04705000	2.22155000
H	-3.44963400	0.32841100	1.49224500
C	-0.86801400	-1.40026900	2.86214900
H	-0.20399200	-2.23278100	2.64584300
C	-1.84766600	-1.02237500	1.94597300
H	-1.94995100	-1.55810300	1.00564500

THFCaCl_anion

Final Single point energy: -6262.946852872483

P	6.58810100	2.68714400	11.24093000
C	5.97784200	1.95511000	9.71242100
C	6.92194800	4.44222300	10.96347000
C	5.35676600	2.48254100	12.55060600
C	4.01902500	2.23782500	12.22805100
H	3.70567000	2.13214300	11.19424200
C	4.98599100	2.63013600	8.98924100
H	4.64985000	3.61893500	9.29127700
C	5.75149900	2.60269000	13.88972000
H	6.79375000	2.77135400	14.14724900
C	7.31343900	4.87505300	9.69280100
H	7.37953800	4.17441700	8.86674700
C	6.84212100	5.34813900	12.02536900
H	6.52354200	5.02319400	13.01113600
C	8.03246400	0.62901600	12.41928000
H	7.06818700	0.18212300	12.64630700
C	7.61388600	6.21636700	9.48643300

H	7.90246300	6.55377400	8.49517300
C	7.15907900	6.68427800	11.81081700
H	7.09316100	7.38929700	12.63394400
C	7.53882000	7.11973300	10.54314800
H	7.77152300	8.16781000	10.37787500
C	8.10774400	1.86572000	11.76686900
C	9.34810600	2.44235100	11.47972800
H	9.40694500	3.40481000	10.97991600
C	4.88237500	0.78056700	7.44794400
H	4.45153300	0.32481900	6.56032500
C	6.43499100	0.70134300	9.29382100
H	7.21507200	0.18244100	9.84239500
C	3.07821600	2.12514700	13.24574400
H	2.04024900	1.93378300	12.99174700
C	4.43532300	2.03224600	7.86373600
H	3.66141400	2.54738600	7.30449800
C	4.80110900	2.49167500	14.89723500
H	5.10668300	2.58408800	15.93497300
C	9.20357300	-0.02646500	12.77896700
H	9.14794100	-0.98497700	13.28586000
C	5.88619000	0.12226400	8.15407800
H	6.24547500	-0.84659900	7.82041200
C	3.46571700	2.25517000	14.57620600
H	2.72672100	2.16460100	15.36711200
C	10.51324700	1.77719800	11.84640800
H	11.47781100	2.22564600	11.62905800
C	10.44160900	0.54653600	12.49377200
H	11.35408000	0.03214400	12.78112400
Ca	0.28628200	3.51309400	4.39719100
Cl	1.15225000	1.76115600	6.18300000
O	-0.29619400	5.73538200	3.83687900
O	-0.02459500	3.02431000	2.08820400
N	-1.93278000	4.04406200	4.99466600
N	2.17492700	4.92698200	4.11769000
C	-2.48272300	5.19064300	4.48194600
C	-1.62940800	6.11865300	3.83089100
C	3.46689500	7.64723800	6.28119000
C	1.98933800	6.13378700	3.49880300
C	-4.54098500	1.63821400	7.32709300
C	-2.78174500	3.31388300	7.16583900
C	-2.06333400	7.30125900	3.26646500
C	3.98266700	5.18895600	5.75792200
C	3.13288400	6.18470000	6.53123500
H	2.10644700	6.03711300	6.17137200
C	-2.79357900	3.22677100	5.75160900
C	3.00915400	6.96233000	2.98342400
H	4.03109200	6.61860400	3.09883600
C	-3.65635900	2.53756200	7.92218500
H	-3.63720200	2.62167500	9.00692700
C	-3.84485500	5.55572100	4.55154700
H	-4.51448300	4.87958900	5.06953000
C	-4.32725200	6.74147900	3.99470500
C	2.72853500	8.16001500	2.32504400
C	0.66156800	6.59825000	3.32291700
C	3.09974800	5.88270900	8.02732700
C	-2.22553000	5.70074600	7.76951100
C	0.34030100	7.79236400	2.70744100
C	4.24610000	3.63793100	3.90701000
C	3.46429900	4.61218800	4.56789100
C	4.76378300	8.10320900	6.04254400
H	5.57563100	7.38789700	5.94181500
C	4.14680600	3.88291000	1.40914600
C	5.24113500	4.81305400	6.22177600
H	5.61227100	5.24727600	7.14970000
C	2.43624400	8.58742500	6.37681700
H	1.41918600	8.24017900	6.54737400
C	-3.43381200	7.59758100	3.34647200
H	-3.79657300	8.51539800	2.89570100
C	-5.81169900	7.12321200	4.06393300
C	1.39595800	8.56734300	2.20236100
H	1.16269900	9.49815000	1.69572400
C	-1.10355500	8.26631400	2.57656500
C	-4.48936300	1.49584400	5.94363300
H	-5.13426400	0.75990800	5.47064700
C	3.89671400	6.56145500	8.95222900
H	4.57900900	7.33562200	8.61089800
C	-3.63252800	2.26171400	5.15202400
C	2.92268700	5.30790300	10.77406300
H	2.84557300	5.09350000	11.83680300
C	-1.78500000	4.25123000	7.83846000
H	-0.86445500	4.18567600	7.24105700
C	2.21894700	4.90317600	8.50071400
H	1.59494900	4.35761200	7.79488600
C	4.08200500	1.56040700	2.45788500
C	-3.51334000	6.08184300	8.15341800
H	-4.21757800	5.32249400	8.48603600
C	-1.41487400	3.79161200	9.24391100
C	5.49631200	3.27781100	4.41081900
H	6.07309600	2.51198900	3.89394500
C	3.80987100	6.27609600	10.31362500
H	4.43331900	6.82252600	11.01522000
C	-1.33917900	6.68312200	7.32758600
H	-0.33905100	6.39553000	7.00716000
C	5.46841600	4.28566800	1.20106800
H	6.23355800	4.01611700	1.92459200
C	3.73997900	3.03791700	2.60495600
H	2.64407300	3.09951100	2.64377300
C	-5.51348100	0.84382300	8.15761800
H	-5.07188100	0.55215000	9.11605400
H	-5.83457400	-0.06134500	7.63356400
H	-6.41264800	1.43248400	8.37995100
C	-1.61004900	4.57181500	10.38312200
H	-2.04194900	5.56386800	10.29125400
C	2.69282000	9.94827900	6.25299000
H	1.87528900	10.66129000	6.32248800
C	6.02208600	3.86540900	5.55805400
C	-0.83735600	2.52329200	9.39663300
H	-0.66246900	1.91322300	8.51349700
C	-6.37453700	7.23437100	2.63361100
H	-7.44524900	7.47144500	2.66219900
H	-6.24497600	6.28793900	2.09727800
H	-5.86755100	8.01884700	2.06247800
C	-0.48856500	2.04163600	10.65226900
H	-0.04359500	1.05412500	10.74626700
C	-3.53548400	1.98211200	3.65456000
H	-2.96206400	2.81648200	3.22709600
C	3.75960700	10.45708500	2.26088200
H	3.89108300	10.44940600	3.34781400

H	2.79859600	10.93131400	2.03753500
H	4.55149800	11.07488900	1.81949300
C	2.12789500	4.61844200	9.85966400
H	1.42604000	3.86440400	10.20441700
C	-1.47391000	8.36243900	1.07945200
H	-2.50272300	8.71756600	0.95794600
H	-1.38941300	7.37931800	0.60282200
H	-0.80643700	9.05758600	0.55952100
C	3.83220400	9.02429400	1.70068000
C	3.99608500	10.39532300	6.03916200
H	4.20211000	11.45793500	5.94339600
C	5.02742200	9.46707100	5.92739700
H	6.04415800	9.80431400	5.74212000
C	-3.01451800	8.39030000	7.65430300
H	-3.32343500	9.43069000	7.59938800
C	5.81465500	5.03023700	0.07698300
H	6.84793800	5.33351300	-0.07057300
C	3.18043400	4.26110100	0.47682900
H	2.14609500	3.97423000	0.64558500
C	-1.25741400	4.09201900	11.64603800
H	-1.42195700	4.71612500	12.52059500
C	-0.70409500	2.82466200	11.78805000
H	-0.44099500	2.44908400	12.77315700
C	-5.96618600	8.48252000	4.77277200
H	-5.42782100	9.27558000	4.24413400
H	-5.57343100	8.42925000	5.79441400
H	-7.02496700	8.76531400	4.82296800
C	-1.72975000	8.01864700	7.26540500
H	-1.03265300	8.76976200	6.90259000
C	-3.90452000	7.41626300	8.10410700
H	-4.91083900	7.69558400	8.40520900
C	3.60668400	0.67330600	3.43313600
H	3.03571100	1.06152700	4.27482400
C	-1.23372100	9.66370200	3.22342200
H	-0.56328700	10.38016100	2.73905400
H	-0.97705000	9.61324100	4.28728000
H	-2.25610800	10.04242500	3.13201000
C	0.16411200	1.77897000	1.35000500
H	-0.10989700	0.95276600	2.01266900
H	1.22533200	1.69424500	1.07676600
C	4.84173600	5.39681000	-0.85114500
H	5.11162700	5.98721200	-1.72249200
C	5.23550700	8.47406500	1.98335100
H	5.37099600	7.47369400	1.55748500
H	5.43609800	8.42201300	3.05966700
H	5.98331700	9.13522100	1.53072400
C	7.35940900	3.44160300	6.10117200
H	7.23702300	2.73407500	6.93307400
H	7.92832300	4.29853100	6.47898300
H	7.95929500	2.94393200	5.33332800
C	3.51892600	5.01411600	-0.64413400
H	2.74754700	5.30787300	-1.35145800
C	3.63305500	9.07353300	0.17326100
H	4.42391000	9.67463200	-0.29286200
H	2.66774900	9.51949300	-0.08804700
H	3.67007900	8.06467400	-0.25328000
C	-4.89522700	1.99208100	2.97643100
C	-2.71029200	0.72188900	3.38035000
C	-6.64915100	6.09108900	4.82946700
H	-7.69510000	6.41715100	4.85146100
H	-6.30768700	5.98426900	5.86556900
H	-6.61489300	5.10507600	4.35187500
C	-6.59861500	3.21798000	1.75418100
H	-6.92610400	4.13524400	1.27236800
C	3.84979900	-0.69109100	3.33929800
H	3.46363100	-1.35969100	4.10483000
C	4.80597600	1.04113400	1.38478000
H	5.17678300	1.70555600	0.60976900
C	-0.66466600	4.01744200	1.22250700
H	-0.09568700	4.95026500	1.29434400
H	-1.68346400	4.18582300	1.59615900
C	4.58256000	-1.20085600	2.26603700
H	4.77547900	-2.26746600	2.18992000
C	-1.73066900	0.30163800	4.28696500
H	-1.59843800	0.83635500	5.22356700
C	-0.66071000	3.40729700	-0.17198800
H	-1.50565800	3.76157400	-0.76844800
H	0.26556700	3.65664900	-0.70185800
C	5.05758200	-0.32955300	1.29212600
H	5.62572600	-0.71317600	0.44865100
C	-5.73683200	0.87328900	2.96874500
H	-5.39923100	-0.05967400	3.41213500
C	-5.34295100	3.16159100	2.35600600
H	-4.70188000	4.04100300	2.35886100
C	-7.43116800	2.10259200	1.76408400
H	-8.40971500	2.14413200	1.29370100
C	-6.99328000	0.92818900	2.37352900
H	-7.62981800	0.04727800	2.37968100
C	-0.92352800	-0.80140700	4.01609400
H	-0.16623000	-1.09688000	4.73736700
C	-0.72431300	1.90652400	0.12337400
H	-1.74886100	1.60908200	0.36838700
H	-0.36785200	1.28848400	-0.70516800
C	-2.85054600	0.00394600	2.18732800
H	-3.59683100	0.30921900	1.45952100
C	-1.08546200	-1.51648700	2.83282800
H	-0.46233400	-2.38139800	2.62250800
C	-2.05312500	-1.10535900	1.91863500
H	-2.18668600	-1.64732800	0.98590400

THFCaF_anion

Final Single point energy: -4995.350418445947

Ca	0.29522700	3.54074000	4.45285500
Cl	1.19283300	1.86777900	6.30196100
O	-0.31228300	5.76513800	3.86709200
O	0.02275600	3.07366300	2.12059000
N	-1.93026400	4.06719000	5.03169400
N	2.14777700	4.98616900	4.16208800
C	-2.49431800	5.19721700	4.49959900
C	-1.64887900	6.12869100	3.84241400
C	3.43121700	7.55406700	6.32024900
C	1.96628800	6.17336300	3.51519900
C	-4.50257100	1.62710500	7.36540000
C	-2.77200900	3.33289300	7.20445900
C	-2.09486400	7.29600100	3.25587200
C	3.92224000	5.09588500	5.84423500
C	3.09704300	6.10343700	6.63073900
H	2.05977800	5.95192900	6.30402700

C	-2.78020700	3.24127400	5.79032100
C	2.98144500	6.99456300	2.98025000
H	4.00516600	6.65960100	3.10557700
C	-3.63657500	2.54488900	7.96011200
H	-3.62285100	2.63335500	9.04451600
C	-3.86224800	5.54308500	4.55254400
H	-4.52614400	4.86561300	5.07625800
C	-4.35669800	6.71379300	3.97395800
C	2.69164900	8.17694100	2.29772600
C	0.63516500	6.62669700	3.33311300
C	3.12052000	5.83759900	8.13141400
C	-2.23833300	5.73106100	7.77938900
C	0.30516900	7.80492800	2.69454800
C	4.20426400	3.68568900	3.88451400
C	3.43111400	4.62834700	4.59720200
C	4.73094500	7.98596200	6.05444200
H	5.53586900	7.25781400	5.99468400
C	4.30680600	4.02581900	1.37736000
C	5.12730600	4.60797300	6.34134900
H	5.47702700	4.95387100	7.31323600
C	2.40789900	8.50511400	6.36955100
H	1.38873000	8.17692300	6.56218500
C	-3.47045100	7.57326600	3.32030700
H	-3.84234200	8.47971100	2.85400200
C	-5.84684800	7.07588000	4.02648200
C	1.35608200	8.57504700	2.16976500
H	1.11591000	9.49199300	1.64147700
C	-1.14272300	8.26591400	2.56094500
C	-4.44413700	1.47974400	5.98264900
H	-5.07488000	0.73135400	5.50982000
C	3.96039300	6.52604500	9.00984000
H	4.61879400	7.30239400	8.62924900
C	-3.59905000	2.25886600	5.19133000
C	3.10326200	5.26059900	10.88167600
H	3.09163900	5.04126600	11.94606100
C	-1.78874300	4.28614600	7.87500000
H	-0.86116200	4.21811800	7.28817900
C	2.26728900	4.85921700	8.65308500
H	1.60911100	4.31099000	7.98143000
C	3.87448500	1.71030000	2.32363200
C	-3.53527400	6.10889300	8.13420000
H	-4.23999700	5.34956300	8.46591600
C	-1.42614700	3.85323200	9.29096900
C	5.40175300	3.20962200	4.42213500
H	5.96293100	2.45257100	3.87582600
C	3.95685100	6.23595200	10.37356300
H	4.61907300	6.78236600	11.04028100
C	-1.34958200	6.71270400	7.34148600
H	-0.34121200	6.42504300	7.04837600
C	5.66316000	4.34929600	1.30125700
H	6.33215000	4.06119600	2.10739400
C	3.72369500	3.21398900	2.52258600
H	2.64405500	3.42150900	2.50360300
C	-5.46247700	0.81846100	8.19696500
H	-5.01136700	0.52365300	9.15007700
H	-5.77932000	-0.08576900	7.66869600
H	-6.36494100	1.39769500	8.43055500
C	-1.61626100	4.66072200	10.41193100
H	-2.04301100	5.65268000	10.29709500
C	2.67419300	9.85495800	6.16807200
H	1.86247100	10.57724600	6.20187500
C	5.88529000	3.66156200	5.64697200
C	-0.85583800	2.58569800	9.47313600
H	-0.68451800	1.95401200	8.60487600
C	-6.40265000	7.15196200	2.59114800
H	-7.47557000	7.38037200	2.60905100
H	-6.26236100	6.19605200	2.07410100
H	-5.89890900	7.92887400	2.00690700
C	-0.50817400	2.13235900	10.73917500
H	-0.06579900	1.14626400	10.85526800
C	-3.49127000	1.98018200	3.69415500
H	-2.96462700	2.84224100	3.26144000
C	3.69909200	10.48452500	2.12002900
H	3.82813500	10.54150800	3.20602400
H	2.73413200	10.93518100	1.86749700
H	4.48541200	11.08521300	1.64627300
C	2.25525700	4.57361700	10.01424100
H	1.57191700	3.82099000	10.39762500
C	-1.51415500	8.35283500	1.06361500
H	-2.54549400	8.69986200	0.94016700
H	-1.42238500	7.36844500	0.59088200
H	-0.85214400	9.05082400	0.54065800
C	3.78948100	9.02427700	1.63950400
C	3.97956100	10.27902500	5.92244100
H	4.19301100	11.33318700	5.76754400
C	5.00459900	9.33875500	5.86210600
H	6.02361600	9.65778800	5.65829800
C	-3.04229200	8.41274300	7.60778500
H	-3.35703900	9.45001000	7.53036200
C	6.16744500	5.04305300	0.20359000
H	7.22571600	5.28771600	0.16218700
C	3.46703500	4.42832900	0.33658700
H	2.40554700	4.19891400	0.39707800
C	-1.26261900	4.20961600	11.68532200
H	-1.41919700	4.85650200	12.54463600
C	-0.71421900	2.94371700	11.85635100
H	-0.44039000	2.59252600	12.84757400
C	-6.02464200	8.44622600	4.70841500
H	-5.49519600	9.23698200	4.16752300
H	-5.63594000	8.41793300	5.73260600
H	-7.08768000	8.71451700	4.74855900
C	-1.74723700	8.04430300	7.25050000
H	-1.04779400	8.79460700	6.89045700
C	-3.93391900	7.43994300	8.05699100
H	-4.94731900	7.71730600	8.33549800
C	3.27080700	0.85390600	3.25369000
H	2.76270500	1.27360500	4.12058300
C	-1.28430500	9.66507200	3.20159900
H	-0.61895400	10.38427100	2.71389600
H	-1.02688500	9.62133000	4.26562100
H	-2.31023500	10.03424400	3.10869400
C	0.28667700	1.87431400	1.33517800
H	0.06851000	1.00904100	1.96729000
H	1.34872300	1.86351600	1.05302600
C	5.32195700	5.43066500	-0.83350300
H	5.71557800	5.97821500	-1.68563200
C	5.19704500	8.50406000	1.95554800
H	5.34922900	7.48996700	1.56944500

H	5.38867800	8.49568500	3.03451700
H	5.94072900	9.15615600	1.48320600
C	7.16216700	3.11877400	6.23226300
H	6.95338100	2.40219400	7.03658300
H	7.77344000	3.91871900	6.66368300
H	7.75636600	2.60199100	5.47292700
C	3.96501100	5.12383300	-0.76122000
H	3.29135600	5.43305600	-1.55620100
C	3.59693500	8.98808800	0.11036100
H	4.38455200	9.56885200	-0.38634800
H	2.62807300	9.40917400	-0.17792300
H	3.64598900	7.95653900	-0.25590100
C	-4.85419100	1.91504000	3.02680000
C	-2.60148900	0.76537400	3.41704200
C	-6.67473000	6.04749200	4.80729700
H	-7.72553600	6.35843500	4.81566300
H	-6.33876400	5.96720300	5.84758400
H	-6.62264200	5.05248500	4.35068900
C	-6.64930300	3.05610000	1.85476200
H	-7.04019700	3.96120300	1.39742400
C	3.31323700	-0.52479200	3.09071000
H	2.83105600	-1.16722500	3.82340400
C	4.53059800	1.14478700	1.22984700
H	5.00254000	1.78663300	0.49148600
C	-0.58356700	4.09331600	1.26016300
H	0.00324800	5.01358500	1.34806600
H	-1.60107800	4.27696400	1.62890900
C	3.97201800	-1.08168400	1.99342100
H	4.00865500	-2.15995100	1.86424400
C	-1.61170300	0.38072000	4.32819400
H	-1.51441700	0.90714900	5.27387600
C	-0.57689100	3.50761900	-0.14696500
H	-1.42981300	3.85969200	-0.73332700
H	0.34308700	3.78296600	-0.67481300
C	4.58185200	-0.24123200	1.06830400
H	5.10017600	-0.66113600	0.21008500
C	-5.62661700	0.74761900	3.01217300
H	-5.22643900	-0.16886300	3.43788700
C	-5.38209300	3.06527600	2.43410200
H	-4.79419400	3.98109700	2.44094200
C	-7.41257400	1.89191600	1.85692600
H	-8.40014400	1.88214700	1.40393400
C	-6.89366600	0.73576400	2.43701300
H	-7.47567800	-0.18213900	2.43799200
C	-0.75236000	-0.68166500	4.05361600
H	0.01108100	-0.94895000	4.77923600
C	-0.60901000	1.99980200	0.11569500
H	-1.62536000	1.67215500	0.35708000
H	-0.23907400	1.40825000	-0.72642600
C	-2.69701300	0.05501500	2.21500600
H	-3.44950200	0.33531300	1.48336800
C	-0.87243600	-1.39239700	2.86293200
H	-0.20867900	-2.22601900	2.65010400
C	-1.84954200	-1.01571600	1.94369300
H	-1.95014800	-1.55347900	1.00434800

THFCaF

Final Single point energy: -5902.594770793938

P	6.08107400	2.59642800	11.34781800
C	5.19690400	1.99597300	9.89365200
C	6.81018100	4.20776900	10.97515900
C	4.97323000	2.78092800	12.76454800
C	3.61964300	3.06549700	12.56395800
H	3.19783100	3.08916000	11.56313200
C	4.40432100	2.88392100	9.15465800
H	4.35011000	3.93608300	9.42122500
C	5.50631300	2.74450500	14.05949500
H	6.55762200	2.52176500	14.21895000
C	7.24466800	4.48705600	9.67624100
H	7.10883200	3.75941100	8.88274600
C	6.98117900	5.14836300	11.99585800
H	6.63313600	4.94316900	13.00362800
C	7.04914300	0.25720600	12.48738700
H	6.02156800	0.06530600	12.78493300
C	7.84552000	5.70989200	9.40136300
H	8.17216500	5.93167500	8.38969200
C	7.59188700	6.36406200	11.71151600
H	7.72030000	7.09681400	12.50238200
C	8.02033500	6.64658500	10.41656300
H	8.48673100	7.60266800	10.19680400
C	7.38403400	1.42914000	11.79738800
C	8.70680700	1.67728400	11.42181500
H	8.96931600	2.58942400	10.89397400
C	3.76272300	1.06971700	7.69973100
H	3.19239200	0.72161500	6.84318900
C	5.28253500	0.64787500	9.52617300
H	5.90984300	-0.04132700	10.08250700
C	2.80760200	3.32934900	13.66174900
H	1.75926200	3.56425700	13.50642700
C	3.68594300	2.41127700	8.06315300
H	3.06640100	3.08872100	7.48567500
C	4.68119100	2.99815000	15.14843400
H	5.09316700	2.96628000	16.15239100
C	8.04335700	-0.66329200	12.79460000
H	7.78630500	-1.57197300	13.33031700
C	4.56413200	0.19203200	8.42623400
H	4.63519100	-0.85234600	8.13728400
C	3.33496600	3.29623400	14.94972900
H	2.69402400	3.50117100	15.80233900
C	9.69365000	0.74877500	11.73656200
H	10.72282700	0.94201000	11.44984800
C	9.36334200	-0.41802800	12.42047800
H	10.13772200	-1.13867700	12.66699700
Ca	0.44674500	3.55190400	4.39865200
F	1.21085000	2.15452800	5.79427100
O	-0.24844600	5.81259900	3.90060900
O	0.10518200	3.11651600	2.05640400
N	-1.79949200	4.01868500	5.00059200
N	2.24076600	5.08857800	4.09359900
C	-2.39961900	5.16579500	4.56200100
C	-1.59294000	6.14523500	3.92511900
C	3.68942800	7.83275900	6.05405600
C	2.00351800	6.26788700	3.45050000
C	-4.08962500	1.35871600	7.38397100
C	-2.49179000	3.18407000	7.18318000
C	-2.08339800	7.32538300	3.40329600
C	4.08559400	5.32710700	5.69354200
C	3.29993700	6.40690000	6.42083300

H	2.25985900	6.27696700	6.09549000
C	-2.57862000	3.14086500	5.76984500
C	2.97349000	7.09002400	2.83987400
H	4.00522100	6.76026600	2.89749500
C	-3.24132000	2.30534000	7.96043400
H	-3.15159900	2.34735400	9.04456100
C	-3.76919400	5.48423300	4.69004200
H	-4.40032700	4.76462500	5.19855400
C	-4.30435400	6.67398500	4.19216100
C	2.62846000	8.25805400	2.15807300
C	0.65652800	6.69745500	3.33703500
C	3.28804400	6.25701300	7.93832200
C	-2.13671700	5.57001300	7.93686600
C	0.27723200	7.87394200	2.72203800
C	4.26682100	3.75511000	3.84609600
C	3.53385200	4.76515900	4.51036500
C	4.98585000	8.19368300	5.68882400
H	5.74460700	7.42372200	5.57454100
C	4.31270000	3.98098300	1.33802700
C	5.30330400	4.85591400	6.17988000
H	5.69950200	5.27166400	7.10544900
C	2.72055400	8.83543400	6.16845800
H	1.70259600	8.56051500	6.44047900
C	-3.45931300	7.57686700	3.54070200
H	-3.86594500	8.49584000	3.13109900
C	-5.79661600	7.00598600	4.32307400
C	1.28554800	8.65026200	2.12670900
H	1.00265500	9.56139500	1.60947900
C	-1.18044500	8.32350700	2.68273300
C	-4.11871900	1.27325600	5.99489200
H	-4.73007100	0.50316100	5.53086900
C	4.27164200	6.82465900	8.75446600
H	5.09220800	7.37850500	8.30523300
C	-3.37232700	2.13088500	5.18551400
C	3.12573500	6.05727000	10.73819100
H	3.05806000	5.99200400	11.82079100
C	-1.53476700	4.18101100	7.82418700
H	-0.69883000	4.27909800	7.11981600
C	2.23005600	5.57824000	8.55010400
H	1.45810700	5.12647400	7.93124000
C	3.88744500	1.70417300	2.40604600
C	-3.42811000	5.77473800	8.42890700
H	-4.02622600	4.91949100	8.73472200
C	-0.94804300	3.62673900	9.11274700
C	5.46991400	3.29410000	4.37784100
H	5.99697700	2.48564900	3.87253000
C	4.19441700	6.72179600	10.14085100
H	4.96674500	7.17500200	10.75586500
C	-1.39916700	6.67764300	7.51293000
H	-0.40324700	6.52959800	7.09964100
C	5.67610800	4.25719100	1.20673400
H	6.36663700	3.94800900	1.98648000
C	3.74707100	3.21539200	2.52466700
H	2.66958200	3.43152700	2.51462000
C	-4.93414900	0.45386900	8.24092400
H	-4.39418600	0.14179400	9.14090600
H	-5.23913800	-0.44165900	7.69139300
H	-5.84721500	0.96518500	8.57147200
C	-1.36655100	4.01497800	10.38522300
H	-2.11106400	4.79898600	10.49354100
C	3.04122700	10.16764700	5.93461000
H	2.27273000	10.93167200	6.01857300
C	6.00967100	3.83280400	5.54266900
C	0.03213800	2.63160000	8.99969400
H	0.38102200	2.34186400	8.00832700
C	-6.41303200	7.14317500	2.91696500
H	-7.48679900	7.35594300	2.98996600
H	-6.28355500	6.21361400	2.35125300
H	-5.94316900	7.95311600	2.34987300
C	0.55547800	2.01790500	10.13126800
H	1.31636900	1.24825000	10.02456000
C	-3.31604200	1.89753100	3.67898000
H	-2.81362400	2.77970900	3.25759900
C	3.63654500	10.55313600	1.85302000
H	3.87084400	10.62297600	2.92049300
H	2.65582200	11.01120200	1.68967800
H	4.37857800	11.13950400	1.29700400
C	2.14385600	5.47937800	9.93633400
H	1.30539100	4.95289300	10.38495000
C	-1.63824600	8.43687400	1.21092300
H	-2.67905600	8.77183700	1.15311000
H	-1.56027100	7.46258200	0.71536000
H	-1.01665800	9.15391600	0.66494800
C	3.66711900	9.08585000	1.38914000
C	4.34530000	10.52159100	5.58851400
H	4.59968700	11.56219100	5.40631600
C	5.31293600	9.52953700	5.46089100
H	6.32813100	9.79387200	5.17598500
C	-3.22116400	8.15516500	8.07674900
H	-3.64549900	9.15448500	8.12152800
C	6.16074500	4.93079000	0.08841700
H	7.22445400	5.13803300	0.00474400
C	3.44826900	4.40810400	0.32825600
H	2.38245000	4.21893700	0.42946100
C	-0.84524400	3.39544600	11.52258400
H	-1.19187800	3.70058100	12.50668600
C	0.10620900	2.38729500	11.39957500
H	0.49804100	1.89093200	12.28294300
C	-5.96782500	8.33571900	5.08184800
H	-5.47219000	9.16214100	4.56254100
H	-5.53825300	8.26089300	6.08743900
H	-7.03227000	8.58327000	5.17765700
C	-1.93527500	7.96074600	7.57758100
H	-1.35105200	8.80809300	7.22773100
C	-3.96484700	7.05711300	8.50497000
H	-4.97305300	7.19804500	8.88590500
C	3.29840500	0.90448500	3.39545800
H	2.78965800	1.37381300	4.23798700
C	-1.29506700	9.70667500	3.36090100
H	-0.67090800	10.44366800	2.84571000
H	-0.96694200	9.64480400	4.40435100
H	-2.32871500	10.06557100	3.34414700
C	0.32761300	1.93168800	1.23863500
H	0.11497500	1.05599200	1.85742500
H	1.38117900	1.91068000	0.92540600
C	5.28886300	5.34609500	-0.91609800
H	5.66735800	5.87895700	-1.78421600
C	5.09295400	8.55411800	1.57829600

H	5.19451600	7.53023600	1.20143800
H	5.39002200	8.56588000	2.63314000
H	5.79370600	9.18627000	1.02091500
C	7.28654200	3.28195700	6.11852600
H	7.07758200	2.51413400	6.87676800
H	7.88542500	4.06543600	6.59441800
H	7.89768100	2.81049200	5.34274300
C	3.92699400	5.08415500	-0.79080400
H	3.23366300	5.41310800	-1.56041100
C	3.33079300	9.02654100	-0.11459900
H	4.07001500	9.59422900	-0.69372700
H	2.34034900	9.44716400	-0.31747600
H	3.34016000	7.98860400	-0.46682900
C	-4.69949100	1.84005800	3.05673700
C	-2.41528100	0.70548600	3.34874300
C	-6.57558700	5.92364700	5.08088700
H	-7.62860800	6.21815200	5.15362500
H	-6.19220600	5.78871700	6.09887700
H	-6.53222800	4.95725700	4.56540800
C	-6.53638100	3.00818000	1.97896600
H	-6.94320600	3.92420700	1.55892200
C	3.35477500	-0.48166700	3.31680500
H	2.88821000	-1.08331200	4.09285300
C	4.53090900	1.07760100	1.33879200
H	4.98768700	1.67765700	0.55701100
C	-0.53373100	4.15530500	1.24577100
H	0.05063900	5.07673700	1.34177800
H	-1.54044300	4.32354600	1.65044700
C	4.00396700	-1.10054600	2.24728500
H	4.04899400	-2.18444000	2.18538800
C	-1.36613100	0.35364700	4.20667800
H	-1.23106900	0.89121600	5.14157900
C	-0.57003500	3.60832300	-0.17609100
H	-1.43690300	3.97979300	-0.72901600
H	0.33656500	3.89252000	-0.72233000
C	4.59064100	-0.31511200	1.26102500
H	5.09823900	-0.78354200	0.42173700
C	-5.47137500	0.67246700	3.04184300
H	-5.05653100	-0.25431200	3.42939400
C	-5.24918600	3.00411800	2.51177400
H	-4.66187600	3.92037000	2.51993200
C	-7.29845900	1.84306700	1.98013800
H	-8.30184100	1.84296400	1.56330200
C	-6.75847800	0.67368500	2.51231000
H	-7.33979100	-0.24465300	2.51097000
C	-0.49482300	-0.68613700	3.89152200
H	0.31302100	-0.92963200	4.57627100
C	-0.60360700	2.09421500	0.04954300
H	-1.61506400	1.76754300	0.31358300
H	-0.26445800	1.52175500	-0.81826200
C	-2.55526500	-0.01281500	2.15659000
H	-3.35171900	0.24400800	1.46405000
C	-0.65821300	-1.40613300	2.71090100
H	0.01657800	-2.22189700	2.46576500
C	-1.69245600	-1.06075500	1.84385500
H	-1.82782100	-1.60590900	0.91324700

THFCa

Final Single point energy: -4534.963311928764

Ca	0.00741200	3.47763000	3.96316900
O	-0.38822600	5.75412900	3.92312600
O	-0.33260400	3.78093400	1.65986200
N	-2.01399000	4.06969600	5.05971600
N	2.02714300	4.70207500	3.86446000
C	-2.54677600	5.27212400	4.65867700
C	-1.69703600	6.19951500	4.00975300
C	3.05277000	7.56420900	5.93062000
C	1.84779700	5.93579800	3.26593600
C	-4.63115300	1.63922400	7.35505500
C	-2.85350300	3.30222400	7.23202000
C	-2.11030800	7.41077100	3.49524400
C	3.67728900	5.10587600	5.63412400
C	2.74850900	6.11720000	6.29012800
H	1.73923200	5.90410800	5.91161300
C	-2.87787900	3.25621200	5.82339600
C	2.86305400	6.69220600	2.65135600
H	3.87028800	6.29294000	2.69146700
C	-3.73164100	2.50537400	7.97022400
H	-3.69842200	2.55113800	9.05701600
C	-3.89037700	5.67609600	4.80778000
H	-4.56062300	5.00092200	5.32641000
C	-4.35347700	6.90071500	4.32143600
C	2.60212100	7.90753500	2.01344500
C	0.55341900	6.50774300	3.24358100
C	2.69977100	5.92523500	7.80444000
C	-2.30213200	5.64308500	8.00457100
C	0.25106900	7.72571800	2.66614300
C	4.20697000	3.53586200	3.86022800
C	3.30023600	4.46193700	4.42044700
C	4.34621800	8.02383000	5.67953200
H	5.17211100	7.31825500	5.65364000
C	4.92788900	3.20745000	1.48154100
C	4.88793000	4.79613200	6.24331200
H	5.13720500	5.27476200	7.18946100
C	2.00676900	8.49089500	5.94607200
H	0.99236700	8.14135100	6.12729000
C	-3.46181000	7.75307300	3.66185300
H	-3.81427000	8.69900700	3.26410900
C	-5.82382500	7.31622500	4.46256400
C	1.29618000	8.40762900	2.02410500
H	1.07809100	9.35392600	1.54085600
C	-1.14238300	8.34678000	2.77461400
C	-4.59883600	1.54331600	5.96238500
H	-5.26223200	0.83952000	5.46508400
C	3.28199400	6.82424800	8.69987400
H	3.77382000	7.71642800	8.32310900
C	-3.73806400	2.32604100	5.19833700
C	2.61234800	5.45554600	10.57456100
H	2.57472700	5.27319800	11.64521200
C	-1.84035100	4.19983100	7.92779600
H	-0.95328300	4.20712400	7.27831300
C	2.06545600	4.78920500	8.31992700
H	1.60156600	4.07981600	7.63563700
C	3.70101000	1.33246400	2.66940700
C	-3.58721200	5.97713600	8.43677600
H	-4.28245700	5.18768200	8.71306700
C	-1.39336900	3.61918600	9.26238100
C	5.41973100	3.26192400	4.50100000

H	6.09861000	2.53828400	4.05557000
C	3.24169300	6.59044300	10.07447000
H	3.70344200	7.30274100	10.75328900
C	-1.42867300	6.66870200	7.64036800
H	-0.42662600	6.41571300	7.29821800
C	6.13249000	2.50808200	1.34590700
H	6.32749400	1.64216900	1.97290800
C	3.89620700	2.83997000	2.54308900
H	2.93972100	3.26155700	2.20956600
C	-5.60881200	0.82797700	8.16233400
H	-5.24325200	0.66445200	9.18054500
H	-5.79503000	-0.14595500	7.69883000
H	-6.57535700	1.34215100	8.23829300
C	-1.54710200	4.28254300	10.47829200
H	-2.00607500	5.26657900	10.50097200
C	2.24460000	9.84348000	5.72602200
H	1.41631700	10.54722300	5.73785900
C	5.78344000	3.87705600	5.69133200
C	-0.78499300	2.35682200	9.26337400
H	-0.65507200	1.83045700	8.31938700
C	-6.45530600	7.41541500	3.05997200
H	-7.51195700	7.69998800	3.13649900
H	-6.39445300	6.44973300	2.54417300
H	-5.94445700	8.16261200	2.44390200
C	-0.35430700	1.77011100	10.44617600
H	0.11718700	0.79105000	10.42380400
C	-3.62651900	2.14541800	3.69421500
H	-3.50606200	3.15202900	3.26587100
C	3.65902900	10.16735300	1.57622900
H	3.78980200	10.33280600	2.65112400
H	2.71646700	10.63088400	1.27005300
H	4.46853300	10.68286800	1.04602700
C	2.02112700	4.55469900	9.68926800
H	1.51300500	3.67329700	10.06856700
C	-1.68333400	8.65366900	1.36143500
H	-2.65934500	9.14544800	1.41738400
H	-1.79557800	7.73045300	0.78306400
H	-1.00209500	9.31916000	0.82236700
C	3.69889500	8.66288200	1.25150400
C	3.54178600	10.29454800	5.48782000
H	3.73168900	11.35049900	5.31561000
C	4.58961500	9.37820700	5.46028000
H	5.60370200	9.71729400	5.26463000
C	-3.11362700	8.32501300	8.12981600
H	-3.43151500	9.36329000	8.17008200
C	7.07718100	2.89157600	0.39910800
H	8.00666200	2.33520000	0.31145400
C	4.69094100	4.28894500	0.63028200
H	3.75991200	4.84364400	0.72011100
C	-1.11214500	3.69770000	11.66902400
H	-1.23956300	4.23270600	12.60640200
C	-0.51821300	2.44061400	11.65987200
H	-0.17983800	1.98583600	12.58679500
C	-5.91641200	8.68684800	5.15950800
H	-5.40225600	9.46717000	4.59000900
H	-5.46463200	8.64073900	6.15683100
H	-6.96634300	8.98457100	5.26856700
C	-1.83010700	8.00100200	7.69638700
H	-1.14132400	8.78757500	7.39833300
C	-3.98942300	7.30785400	8.50543900
H	-4.99411000	7.55148300	8.84102100
C	3.51128400	0.70897000	3.90438200
H	3.52203600	1.30487300	4.81297300
C	-1.04212600	9.66683000	3.57252800
H	-0.34807200	10.36134400	3.08799200
H	-0.68225900	9.46991100	4.58764800
H	-2.02285300	10.14893400	3.63957300
C	0.71887900	3.59571800	0.66637700
H	1.12868400	2.58745000	0.79249600
H	1.49900700	4.34469200	0.85559100
C	6.83232900	3.97787300	-0.43965500
H	7.56812700	4.27348400	-1.18232700
C	5.10399500	8.14818600	1.59193800
H	5.24420200	7.10565100	1.28801700
H	5.30650200	8.22566700	2.66646800
H	5.84962800	8.74962200	1.05997400
C	7.09021400	3.57159800	6.37310100
H	6.93072500	3.25497700	7.41029200
H	7.73673300	4.45687200	6.40422800
H	7.63234700	2.77651600	5.85331000
C	5.63217100	4.67281100	-0.32305300
H	5.42415500	5.51646500	-0.97603400
C	3.45937000	8.46815800	-0.25914800
H	4.23535300	8.98166700	-0.84057000
H	2.48406100	8.86950700	-0.55559800
H	3.48257100	7.40289800	-0.51833500
C	-4.87873400	1.55934500	3.07238600
C	-2.35550000	1.38899700	3.30970400
C	-6.64238000	6.31267500	5.28482300
H	-7.67458200	6.67017300	5.36888300
H	-6.24015200	6.19941700	6.29807800
H	-6.66860900	5.32437600	4.81169800
C	-7.10049200	1.91695800	2.16872100
H	-7.89360200	2.60021100	1.87705100
C	3.33167400	-0.67200800	3.98975000
H	3.19387800	-1.13509100	4.96342500
C	3.67303800	0.53649200	1.51585500
H	3.80596700	1.00232400	0.54258000
C	-1.46674600	4.46614000	1.04211200
H	-1.77462700	5.28508100	1.69973200
H	-2.28949400	3.74590700	0.95008500
C	3.33794400	-1.45480100	2.84012000
H	3.20983700	-2.53162400	2.90721800
C	-1.41566000	0.96428200	4.25788100
H	-1.62620700	1.08696300	5.31764300
C	-0.96475000	4.92456400	-0.31857300
H	-1.77869100	5.01805100	-1.04220900
H	-0.45570000	5.89182300	-0.23197400
C	3.50274600	-0.84083400	1.59834100
H	3.49614200	-1.43777800	0.69005800
C	-5.05408400	0.18360500	2.90817000
H	-4.25707400	-0.49867800	3.19434100
C	-5.91383700	2.41887600	2.69499200
H	-5.78459400	3.49278800	2.81897400
C	-7.26792100	0.54235900	2.01070900
H	-8.19181700	0.14778600	1.59707000
C	-6.24055500	-0.32201800	2.38188800
H	-6.36219500	-1.39517500	2.26163700

C	-0.20564200	0.38753600	3.85915700
H	0.51263100	0.06634400	4.60954600
C	0.04338600	3.82825400	-0.67317000
H	-0.47426200	2.92088100	-1.00560700
H	0.75874200	4.13070600	-1.44251000
C	-2.08151000	1.15197100	1.95751400
H	-2.81489100	1.44215800	1.20906100
C	0.07121000	0.20362900	2.50558200
H	1.01406400	-0.23624000	2.19740100
C	-0.88483800	0.56806800	1.55889700
H	-0.68842100	0.41048500	0.50177500

THFCaTHF

Final Single point energy: -4767.389392289083

Ca	4.87050000	8.95657500	12.95280400
O	4.73281700	7.75087000	14.97204200
O	4.96657700	10.58853000	11.26800000
N	6.80792200	9.26551100	14.29658900
N	2.65329500	8.28246300	13.43998200
C	7.86508000	10.18756700	14.11756400
C	8.12820600	8.29677300	16.14818200
H	8.98963900	8.87456900	15.83610700
C	0.76498100	9.59928300	12.57545600
C	6.95012900	8.42987500	15.38045100
C	1.56061400	8.42949400	12.55948400
C	7.93630700	11.36380200	14.91071700
C	-0.28906000	9.74349700	11.67318200
H	-0.87171400	10.66304900	11.68512300
C	2.42740800	7.52060100	14.56061800
C	8.21157800	7.44402400	17.24849000
C	0.24868200	10.44035900	14.88728300
C	5.87706600	6.80960200	16.90154700
C	5.85321200	7.62939100	15.78837400
C	1.03464000	10.68392700	13.60795900
H	2.09561700	10.59348300	13.88207500
C	1.17302400	7.01619600	14.96613200
H	0.31832500	7.26085800	14.34651300
C	0.85198900	12.08818400	13.04178100
C	8.98111900	12.26487500	14.73533100
H	9.03382400	13.14366700	15.37633400
C	3.42216000	6.41512900	16.52895900
C	1.26412600	7.43505900	11.59362800
C	9.50593100	7.28845000	18.05802000
C	9.89178900	10.92585300	12.98677800
H	10.64513800	10.76093700	12.21923600
C	9.96730000	12.07370400	13.76501700
C	-0.60501800	8.75380500	10.74520900
C	8.87819700	9.97733000	13.15946000
C	1.01899200	6.23974900	16.11352900
C	1.51529400	12.42092500	11.85398200
H	2.10085600	11.65578500	11.34805100
C	-1.14533300	10.33961200	14.87744200
H	-1.68238600	10.39962500	13.93441600
C	0.19466100	7.61343500	10.71564200
H	0.00264900	6.85920700	9.95481500
C	0.91457300	10.33524100	16.10891100
H	2.00103200	10.36618300	16.12769300
C	-0.35202300	5.72384100	16.57235400
C	3.52326500	7.20550400	15.40016500
C	2.15028500	5.93393200	16.87562900
H	2.05103100	5.30784400	17.75559300
C	2.52731100	5.85072200	10.05516200
C	7.07824700	6.71822000	17.62189500
H	7.12027100	6.06202700	18.48482700
C	6.85282000	11.65879900	15.93977600
H	6.41161400	10.69853400	16.22573000
C	9.91364700	7.70525600	12.91483300
C	0.10375500	13.07863900	13.67859900
H	-0.41027300	12.85383400	14.60827200
C	5.72533900	12.49560200	15.35754600
C	8.90967400	8.69614300	12.34125900
H	7.92259500	8.22854200	12.47198300
C	2.13458000	6.19258800	11.49402500
H	3.06414100	6.45076900	12.01880600
C	1.42551600	13.69824100	11.31495900
H	1.94631300	13.93615900	10.39089600
C	1.56489700	4.98005400	12.21818200
C	0.00868200	14.36207100	13.13865200
H	-0.58205700	15.11608700	13.65226700
C	4.64911700	6.02056200	17.34467600
C	-1.85541200	10.17138000	16.06216700
H	-2.93956100	10.09980900	16.03509500
C	11.29348100	7.90044000	12.79278600
H	11.67202100	8.76705000	12.25788100
C	5.96002100	13.61745300	14.55759800
H	6.97751700	13.87589600	14.27675500
C	0.20909000	10.16614500	17.29785500
H	0.74818400	10.08223600	18.23786500
C	7.43259100	12.26249700	17.21629100
C	-1.47304500	6.10330800	15.59711000
H	-1.57890500	7.19038600	15.50649900
H	-2.42492500	5.70227700	15.96292000
H	-1.29286700	5.68915300	14.59807600
C	2.72880600	4.52975200	9.64112000
H	2.55759800	3.71477900	10.33813400
C	9.94825200	5.81248400	18.04890500
H	9.18374300	5.16041500	18.48277000
H	10.86903100	5.69187900	18.63249500
H	10.14379100	5.47577200	17.02507800
C	-1.18090000	10.09306200	17.27929100
H	-1.73514200	9.96137900	18.20458400
C	12.19273400	6.98598200	13.33185500
H	13.26098300	7.15558500	13.22626300
C	-0.68507300	6.32793800	17.95023000
H	0.05494400	6.03455200	18.70213500
H	-1.67022500	5.98342400	18.28903900
H	-0.70136800	7.42147900	17.89593300
C	0.66557500	14.67783300	11.95471700
H	0.59098900	15.67644800	11.53325500
C	4.40526400	12.17604600	15.68545800
H	4.21276700	11.30843700	16.31436300
C	10.65769100	8.12980300	17.49235400
H	10.89368000	7.84666000	16.45973300
H	11.55602900	7.96884500	18.09862900
H	10.42917400	9.20153600	17.51234900
C	-1.77103700	8.91054900	9.80592500
H	-2.69297700	8.52170400	10.25681200
H	-1.60603600	8.36070000	8.87429400

H	-1.94621200	9.96310500	9.56265100
C	0.29826500	4.47541900	11.91506200
H	-0.33438200	4.99490300	11.20083900
C	11.05793700	13.09105700	13.56365400
H	10.68396600	13.96666300	13.01816800
H	11.88944200	12.67262500	12.98921600
H	11.44540400	13.45014100	14.52290500
C	4.90358200	14.40720700	14.11081200
H	5.10683200	15.27606500	13.48992300
C	9.25641000	7.72373800	19.51516200
H	8.91876000	8.76509400	19.55764000
H	10.18065900	7.63680100	20.09925700
H	8.49285100	7.10136500	19.99272600
C	2.75983800	6.87115300	9.12617000
H	2.60690600	7.90491800	9.42424700
C	9.07040200	8.93890700	10.84569600
C	3.34707800	12.96376900	15.23965000
H	2.32675100	12.70264900	15.50424200
C	3.59191700	14.08341500	14.44955300
H	2.76290400	14.68700500	14.09054300
C	9.63387000	7.97180400	10.00753200
H	10.05585700	7.06781700	10.43772200
C	-0.32619900	4.18898100	16.69628800
H	-0.07578400	3.73045800	15.73462800
H	-1.31025100	3.82027600	17.01113200
H	0.40993800	3.85449500	17.43433600
C	9.46159700	6.57083300	13.59007400
H	8.39353100	6.41508100	13.71536600
C	9.65227600	8.14613300	8.62547700
H	10.09333200	7.37897100	7.99444900
C	-0.16028200	3.30091500	12.50571000
H	-1.14808600	2.92253100	12.25579000
C	7.29287200	13.60594500	17.56608900
H	6.72048600	14.27534500	16.93062500
C	11.72836800	5.85124900	13.99663100
H	12.43105200	5.13407900	14.41204100
C	4.64000300	12.11941100	9.49074800
H	4.94964300	12.33210100	8.46406500
H	3.60405800	12.44853500	9.61661300
C	3.16970000	6.58512600	7.82810300
H	3.34182200	7.39893000	7.12805800
C	2.35172800	4.29067000	13.14300800
H	3.32692800	4.68835900	13.41483300
C	5.31263100	11.92174000	11.77079300
H	6.19589000	11.82358000	12.41227500
H	4.46668800	12.28830900	12.36574000
C	8.16048400	11.42369900	18.06895000
H	8.26231100	10.37198100	17.80825900
C	3.13688700	4.23905500	8.34023600
H	3.28064000	3.20337100	8.04367600
C	3.35771700	5.26422500	7.42557700
H	3.67144300	5.03806300	6.41020500
C	0.64474200	2.60710800	13.40672300
H	0.28866000	1.68787600	13.86391300
C	1.90193500	3.11128700	13.73008100
H	2.53103200	2.59229700	14.44881900
C	10.35807400	5.64532800	14.12023400
H	9.98095800	4.76473300	14.63320700
C	5.54962000	12.77698400	10.53475100
H	5.30022200	13.82541800	10.71852600
H	6.59742500	12.71814400	10.22023500
C	7.87979200	14.10329300	18.73062900
H	7.75987100	15.15331200	18.98434600
C	4.91506100	4.51155900	17.13784000
H	5.78911600	4.19207300	17.71568600
H	5.10157100	4.29960800	16.07903800
H	4.04950300	3.92325200	17.46116800
C	8.74657900	11.91662400	19.22859200
H	9.30873100	11.24811800	19.87582700
C	8.61147700	13.26419600	19.56407400
H	9.06756700	13.65207700	20.47073200
C	9.10725500	9.29224700	8.05235800
H	9.12254900	9.42815400	6.97456900
C	4.38504800	6.28897800	18.84218500
H	3.52333300	5.71649600	19.19600100
H	4.18708200	7.35304700	19.00934400
H	5.24582900	5.99810200	19.45058900
C	4.77510000	10.64233300	9.82224300
H	3.88873800	10.04799200	9.57976000
H	5.65825400	10.20431200	9.34171300
C	8.53093300	10.08891500	10.25780900
H	8.08580800	10.84957500	10.89308400
C	8.54691300	10.26519500	8.87770100
H	8.11751900	11.16603400	8.44600600
O	5.55487100	7.24340700	11.49135700
C	5.99847800	7.37473400	10.09751800
C	5.87639300	5.90347200	11.97019300
C	6.47976200	5.98989300	9.69194500
H	5.15047300	7.72442600	9.50539100
H	6.80561800	8.11357300	10.07345500
C	6.95098400	5.40040200	11.02488200
H	6.18563100	5.98576800	13.01801100
H	4.97482300	5.28095800	11.90197300
H	7.27413300	6.04431300	8.94257800
H	5.64768000	5.40227100	9.28789700
H	7.93020500	5.80690100	11.30336300
H	7.00895700	4.30860000	11.01640200

THF

Final Single point energy: -232.393816320879

O	4.83930400	10.94206700	11.50227400
C	4.43973100	10.95248600	9.16127000
H	4.25848800	9.95142000	8.76069700
H	4.04178300	11.67814900	8.44626700
C	5.97814900	11.58619500	10.91510600
H	6.86904900	11.25511700	11.45622300
H	5.88085600	12.68024000	11.01716900
C	5.94898200	11.17110900	9.44042500
H	6.39249900	11.93380100	8.79393300
H	6.50597000	10.24027600	9.29893400
C	3.78459500	11.12336500	10.54523800
H	3.35999100	12.13469600	10.65284700
H	3.00579400	10.38695000	10.76271800

TS_Br_axial2equitoral

Final Single point energy: -6876.878697960657

Ca	-0.75475400	-0.28151700	1.29606700
O	-0.19887000	1.36764200	-0.26228500

Br	-1.91570600	-0.88275700	3.70038400
N	1.45768800	0.33993100	1.54839800
N	-2.15417100	-0.39602600	-0.54530100
C	2.23354200	0.04222300	2.68039200
C	3.38503900	1.42769600	0.43274800
H	4.06277100	0.96366900	1.14060400
C	1.15493900	1.72393900	-0.37517400
C	-0.94400300	1.45057900	-1.44970400
C	-2.94747600	-1.52739400	-0.80861300
C	2.00931500	1.14462500	0.58323600
C	3.86789200	2.23783600	-0.59400800
C	2.45743400	1.01254900	3.69035000
C	2.95352700	2.84333000	-1.46818300
H	3.31144700	3.49891700	-2.25236900
C	-0.62867200	2.37614400	-2.42779400
C	-4.26991300	-1.62648800	-0.32362300
C	2.73965400	3.47930600	3.02977000
C	1.57824600	2.60701200	-1.35213000
C	4.09938700	3.54219100	3.33503100
H	4.55740600	2.74524900	3.91461300
C	-1.96511400	0.49012200	-1.57473600
C	-2.71081800	0.53553900	-2.77436300
H	-3.50433400	-0.19337400	-2.89246200
C	-2.44557200	1.46652700	-3.77698700
C	1.18917300	2.80811600	4.90004600
C	2.17755700	4.50609800	2.26540900
H	1.11942300	4.46277700	2.01380500
C	-5.03435400	-2.75754300	-0.61365400
H	-6.05421200	-2.81428800	-0.23840500
C	-5.30295100	0.68096500	-0.33111600
C	-7.21796900	-0.52885700	1.48819300
H	-7.53975400	0.19070600	0.74120900
C	1.82838400	2.39368200	3.57475800
H	1.00671000	2.28884600	2.85279400
C	2.71220200	-1.27031300	2.90226800
C	4.30542300	5.63628200	2.14698100
H	4.91301600	6.46962600	1.80463800
C	2.35009600	-3.73873800	2.46485900
C	3.43340300	-2.26359200	0.69760900
C	-5.89426300	-0.96778500	1.50478700
C	-4.52079400	-3.82625000	-1.34643700
C	2.45527700	-2.34589800	1.85723400
H	1.46738000	-2.14192500	1.41793100
C	2.95147200	5.57359800	1.82189200
H	2.49741100	6.35784600	1.22170000
C	3.71289300	-0.60226400	5.02077500
C	-4.83789700	-0.48873200	0.51503100
H	-4.00004500	-0.11140300	1.11834700
C	4.87619500	4.61411100	2.90063200
H	5.93435700	4.64671900	3.14746400
C	3.18823300	0.67449700	4.82904300
H	3.32263400	1.42336800	5.60835700
C	-1.39737000	2.38073000	-3.59724400
H	-1.17983500	3.10837200	-4.36974100
C	-5.50970300	-1.88682000	2.49012100
H	-4.47738800	-2.22697600	2.52123900
C	3.44106000	-1.56774500	4.05248000
H	3.79670700	-2.58543200	4.20254400
C	-0.92242200	-2.64021500	-1.85836100
H	-0.44993200	-1.90209900	-1.19087500
C	-2.39554400	-2.64509400	-1.48425400
C	0.51242500	3.34967000	-2.15434000
C	-3.18470800	-3.76356200	-1.74289200
H	-2.73652500	-4.62254000	-2.24062700
C	1.65413200	3.86738500	5.67950300
H	2.50164500	4.45732000	5.34202600
C	0.09062400	2.07215300	5.35952600
H	-0.28052700	1.23905100	4.76568700
C	5.37119800	2.43937600	-0.82711200
C	3.25176900	-4.76406100	2.18582000
H	4.07947600	-4.58512300	1.50549900
C	6.22219600	1.87330600	0.31685600
H	6.09872500	0.78970700	0.41591600
H	5.96647500	2.33985800	1.27486800
H	7.28072500	2.07106000	0.11325700
C	4.79623000	-2.03641600	0.89876600
H	5.17007900	-1.87311300	1.90667100
C	2.96999300	-2.45043600	-0.60535900
H	1.91035500	-2.62832800	-0.77170700
C	-0.62264000	-2.14548900	-3.26189700
C	-3.29020400	1.54540300	-5.05617900
C	1.03980700	4.18001700	6.89373600
H	1.41952000	5.00713700	7.48799000
C	-0.24538400	-3.97362000	-1.55168000
C	-4.94646400	1.98058500	0.03098800
H	-4.30109200	2.13317600	0.89384800
C	-6.12182600	0.49538000	-1.44693000
H	-6.39577800	-0.51338300	-1.74797900
C	-1.36118500	-2.56691300	-4.36823300
H	-2.22404300	-3.21219500	-4.22491700
C	-8.13831500	-1.00200000	2.42570100
H	-9.16510500	-0.64705200	2.39403600
C	-0.05164200	3.44288800	7.34107200
H	-0.53136800	3.68999600	8.28423900
C	1.28497800	-4.00225100	3.33514000
H	0.57331400	-3.20973500	3.56298900
C	4.53551800	-0.93126400	6.23764400
H	4.24081400	-0.31562300	7.09326500
H	5.60197200	-0.74693900	6.05440500
H	4.42942100	-1.98458500	6.51512900
C	-0.52678700	2.38544600	6.56407000
H	-1.38188200	1.80268400	6.89744700
C	-7.74684200	-1.91818500	3.39546300
H	-8.46293900	-2.28436500	4.12604800
C	0.48835700	-4.69014100	-2.49710500
H	0.55442700	-4.32644300	-3.51808000
C	5.67637700	-2.01188000	-0.18039600
H	6.73513200	-1.83693200	-0.00767000
C	3.09601700	-6.02503000	2.76362200
H	3.80844200	-6.81235800	2.53126400
C	-6.42228500	-2.35703500	3.42554200
H	-6.09931500	-3.06550400	4.18398300
C	-6.59012500	1.58697200	-2.17240900
H	-7.23125300	1.42719200	-3.03554000
C	-6.22849700	2.88118000	-1.80356100
H	-6.58561700	3.73275700	-2.37634000
C	-0.02719700	4.49561900	-1.26172700
H	0.78377000	5.18918800	-1.00932800

H	-0.44439900	4.09949900	-0.33034400
H	-0.81511100	5.04565500	-1.78950700
C	-4.29613400	0.39247100	-5.16444200
H	-5.01939700	0.40853500	-4.34232200
H	-3.79095900	-0.58056300	-5.16223500
H	-4.85303800	0.48424400	-6.10369400
C	-0.29849800	-4.46344100	-0.24002900
H	-0.86918900	-3.92076400	0.51232600
C	3.84356100	-2.41279400	-1.68836300
H	3.45832700	-2.54909800	-2.69597300
C	-5.39768500	3.07502800	-0.70247700
H	-5.10120300	4.07972700	-0.41294500
C	5.20383600	-2.19792100	-1.47786300
H	5.89040600	-2.16693100	-2.31957800
C	1.07462600	3.95837900	-3.43993200
H	0.30052600	4.52068800	-3.96953100
H	1.46924200	3.18808500	-4.11128800
H	1.87662600	4.66443700	-3.20664400
C	-4.07180100	2.87403300	-5.05426000
H	-4.69540500	2.95084000	-5.95393200
H	-3.39131600	3.73194600	-5.03540900
H	-4.72191800	2.93463800	-4.17480500
C	5.76405500	1.71183100	-2.12880600
H	6.83910600	1.82355200	-2.31886100
H	5.21885700	2.11935500	-2.98693700
H	5.53506800	0.64255100	-2.05541500
C	5.70622800	3.93528700	-0.97187300
H	5.41044100	4.48579400	-0.07265000
H	5.20152500	4.38791000	-1.83070800
H	6.78610700	4.06214000	-1.11603100
C	2.03468300	-6.27742100	3.62566800
H	1.91078900	-7.26044300	4.07175700
C	-5.36714600	-5.02621300	-1.67815100
H	-5.63724100	-5.03628400	-2.74151200
H	-6.29464100	-5.02935900	-1.09831300
H	-4.82978000	-5.95883300	-1.47432500
C	0.47153500	-1.30185800	-3.46591300
H	1.04479900	-0.95181300	-2.60920300
C	1.15336200	-5.86504600	-2.14176800
H	1.72159500	-6.40621800	-2.89385200
C	-2.38533500	1.50255500	-6.30160200
H	-1.81363800	0.56921100	-6.33130800
H	-1.67643200	2.33596700	-6.31982500
H	-2.99774100	1.56307300	-7.20967200
C	1.12538000	-5.25677100	3.90904600
H	0.28769400	-5.44194000	4.57635200
C	0.36890900	-5.62681400	0.11879300
H	0.33611400	-5.97130100	1.14880800
C	1.10086500	-6.33545600	-0.83454300
H	1.62941900	-7.24240100	-0.55372300
C	-1.00370900	-2.16581600	-5.65292700
H	-1.59031800	-2.50060500	-6.50460700
C	0.82973900	-0.89508400	-4.74787600
H	1.67988600	-0.23178200	-4.88555700
C	0.09622100	-1.33308000	-5.84826100
H	0.37210000	-1.01725500	-6.85074600

TS_Br_CaF

Final Single point energy: -6976.883571764344

Ca	11.15588400	15.59155000	6.20816100
O	11.58150700	17.29589100	4.54755000
F	10.95263900	13.74325900	7.17161800
N	13.42928900	16.22607300	6.16018400
N	9.70916600	15.42287100	4.36929100
C	14.34136600	15.89790400	7.17570900
C	15.19244700	17.51395900	4.99002700
H	15.94648800	17.06286600	5.62462600
C	12.89914300	17.70968500	4.34982200
C	10.74467100	17.35638000	3.43022400
C	8.90600500	14.28897400	4.18835300
C	13.85067400	17.12542700	5.21368700
C	15.55301600	18.41359500	3.98791600
C	14.57513000	16.78686700	8.25580300
C	14.54985800	18.99127900	3.19596500
H	14.81583500	19.70672300	2.42737700
C	10.93703200	18.31389000	2.45222700
C	7.62241100	14.19984300	4.76908000
C	14.43099000	19.30406700	7.78948600
C	13.20379300	18.65271000	3.38407200
C	15.79219600	19.56514400	7.95289400
H	16.42448400	18.83363400	8.44913800
C	9.75949700	16.34812800	3.36480400
C	8.90997400	16.39351900	2.23446900
H	8.14175100	15.63156400	2.16467400
C	9.05562900	17.35330000	1.23422200
C	13.28551700	18.28998300	9.80202900
C	13.64076500	20.25144300	7.13372900
H	12.57870100	20.05475000	6.99894900
C	6.86720900	13.03580000	4.62056100
H	5.88685800	12.97960800	5.09175300
C	6.30642200	16.36977600	4.72289700
C	4.97835300	15.11983600	7.00831600
H	4.39431100	15.63103900	6.24816500
C	13.76457400	18.06930200	8.36877800
H	12.86096800	17.90580100	7.76365600
C	14.97340600	14.63315600	7.21219900
C	15.55357500	21.69040900	6.82928600
H	15.99021000	22.61192400	6.45344100
C	14.72598400	12.18446800	6.68206300
C	15.46404900	13.79527400	4.86727400
C	6.34511400	14.92338900	6.81417200
C	7.34379700	11.93681100	3.90752600
C	14.65388400	13.60486800	6.13747900
H	13.60536500	13.77116000	5.85342400
C	14.19581300	21.43293900	6.65105600
H	13.56638800	22.15352400	6.13536800
C	16.17847200	15.23941400	9.24447600
C	7.09002800	15.37917700	5.56682600
H	7.97282700	15.93001300	5.91893600
C	16.34964900	20.75042600	7.47988700
H	17.41250900	20.93639700	7.61274400
C	15.48601400	16.44881100	9.25593800
H	15.63187300	17.13557900	10.08857700
C	10.07786000	18.30771200	1.34584600
H	10.19884300	19.05959100	0.57525400
C	7.07716500	14.27255200	7.81623900
H	8.14572300	14.11264500	7.67740500
C	15.88044000	14.33259700	8.22866600

H	16.35701300	13.35385000	8.23557400
C	10.86359000	13.17242300	3.03971600
H	11.38289600	13.88224200	3.70109800
C	9.42406400	13.14737100	3.52890100
C	12.04115800	19.34418900	2.67302400
C	8.63815100	12.00515800	3.38998200
H	9.05876800	11.13106500	2.89470000
C	13.61591700	19.41578000	10.55576400
H	14.24580700	20.18827800	10.12435500
C	12.46368400	17.31685100	10.38486600
H	12.19691100	16.43184300	9.81047100
C	17.02200000	18.75170100	3.69723000
C	15.67912700	11.25512900	6.26924700
H	16.40348700	11.52878400	5.50700100
C	17.97586700	18.17090800	4.74929100
H	17.93632400	17.07681200	4.77128000
H	17.74046600	18.54515200	5.75227500
H	19.00420600	18.46393200	4.50863600
C	16.79800800	14.20474400	4.88906800
H	17.26986200	14.44300900	5.83923800
C	14.87108400	13.51047400	3.63515300
H	13.83417400	13.18264100	3.61002300
C	11.03362000	13.72880800	1.63843000
C	8.09732200	17.42409900	0.03694200
C	13.14254900	19.56449700	11.86085500
H	13.41310500	20.44963600	12.43082400
C	11.56103600	11.83041200	3.23043300
C	6.48827200	17.73791200	4.94163100
H	7.21153200	18.06545500	5.68719700
C	5.38855800	15.96117500	3.75348500
H	5.24888500	14.90091900	3.55836200
C	10.21092200	13.33182700	0.58300200
H	9.38179200	12.65474700	0.77496500
C	4.35306500	14.66977800	8.17252400
H	3.28647500	14.83203200	8.30528800
C	12.32636300	18.59244400	12.42824200
H	11.95265100	18.71128000	13.44161800
C	13.79231000	11.80301400	7.65406600
H	13.02791100	12.51586400	7.95769900
C	17.19696700	14.91590400	10.30522600
H	16.94466500	15.39640600	11.25597600
H	18.19488200	15.27008200	10.01576200
H	17.26889700	13.83639300	10.47083100
C	11.98557100	17.46453300	11.68014800
H	11.34070900	16.70077800	12.10661200
C	5.08793300	14.02329300	9.16041500
H	4.60192700	13.67801400	10.06890800
C	12.05118700	11.06411600	2.17271400
H	11.92554200	11.41129800	1.15132400
C	17.52382400	14.32087300	3.70543600
H	18.56149000	14.64309000	3.73913800
C	15.70850200	9.97331400	6.82179300
H	16.45802800	9.26122100	6.48595300
C	6.45810200	13.82859400	8.97773600
H	7.04574700	13.33216300	9.74555000
C	4.65682100	16.89906100	3.02880200
H	3.94605000	16.56407700	2.27756100
C	4.84215000	18.26098200	3.25511400
H	4.27876400	18.99267700	2.68205700
C	11.49175500	20.43809200	3.62405700
H	12.27078100	21.18108400	3.83237900
H	11.16864200	19.99988500	4.57393100
H	10.63316200	20.94042600	3.16320200
C	7.14551800	16.22256800	-0.02271600
H	6.49271600	16.17777500	0.85561500
H	7.69917500	15.27874300	-0.09093000
H	6.50742700	16.30778600	-0.90986700
C	11.75509900	11.36912400	4.53953700
H	11.39646600	11.96889800	5.37613300
C	15.58829100	13.63650000	2.44913900
H	15.10142100	13.42298500	1.50055800
C	5.76599000	18.67769600	4.21158200
H	5.92907800	19.73783600	4.38764700
C	16.92159500	14.04082900	2.48080900
H	17.48501600	14.14400400	1.55729700
C	12.47642600	20.00998200	1.36611500
H	11.63360400	20.53092600	0.90309400
H	12.86951800	19.27743500	0.65268700
H	13.24749000	20.76190000	1.55693700
C	7.25124300	18.70737700	0.15283500
H	6.54361200	18.77504100	-0.68343100
H	7.88516900	19.60035600	0.13933500
H	6.68189500	18.70722600	1.08924900
C	17.40178100	18.16360300	2.32374800
H	18.45465600	18.37338400	2.09526900
H	16.78562300	18.59300000	1.52657300
H	17.25629300	17.07715000	2.31855200
C	17.22991300	20.27746000	3.66387400
H	16.94905100	20.72274100	4.62404800
H	16.63324200	20.75384900	2.87997100
H	18.28453100	20.50847700	3.46895300
C	14.78529700	9.60660100	7.79502000
H	14.80746400	8.60859600	8.22459700
C	6.49578300	10.70733900	3.71496600
H	7.11221000	9.80407600	3.66503100
H	5.92439100	10.76479600	2.77942900
H	5.77573200	10.59081800	4.53092600
C	12.07676400	14.61972700	1.37741000
H	12.71094100	14.95466200	2.19563600
C	12.71445800	9.85966600	2.41340000
H	13.09146100	9.27859400	1.57558500
C	8.88769200	17.46362000	-1.28421800
H	9.50194300	16.56321500	-1.39034900
H	9.54773300	18.33468900	-1.34004600
H	8.19474500	17.51237300	-2.13335500
C	13.82249100	10.52978000	8.20812900
H	13.08578900	10.25022100	8.95710000
C	12.41926700	10.17308200	4.77981500
H	12.58271300	9.84580800	5.80272500
C	12.90107000	9.40963100	3.71583900
H	13.42659400	8.47744000	3.90578100
C	10.44064500	13.79637500	-0.70940400
H	9.79067600	13.47791700	-1.52049100
C	12.30565700	15.09292100	0.08858300
H	13.11723600	15.79334300	-0.09216400
C	11.49232000	14.67507500	-0.96250800
H	11.66814700	15.04247500	-1.97002200
Br	9.24998600	18.64391100	8.00202100

TS_BrCa_F

Final Single point energy: -6976.858702353242

Ca	11.04055000	15.86974700	6.26546900
O	11.55226500	17.37778900	4.54372000
F	10.40701900	12.86460400	7.35836400
N	13.35272200	16.31282400	6.19838200
N	9.73590800	15.45115600	4.36562400
C	14.26381400	15.95797300	7.21037200
C	15.16134700	17.51982200	4.99767800
H	15.90383000	17.07168700	5.64759100
C	12.88086600	17.75256300	4.34110300
C	10.72787400	17.40307400	3.41547600
C	8.94837100	14.30384200	4.17238900
C	13.81054600	17.16746300	5.22571300
C	15.54403700	18.38536100	3.97287100
C	14.51871600	16.83581400	8.29424700
C	14.55804400	18.96382100	3.15907300
H	14.84349900	19.65174700	2.37253800
C	10.92943600	18.34019000	2.42132700
C	7.66732600	14.18992600	4.75121200
C	14.39768600	19.34057600	7.78620000
C	13.20414300	18.66111100	3.35055900
C	15.76321600	19.59655600	7.92219600
H	16.39507300	18.87985400	8.44053300
C	9.76233300	16.37691800	3.35871600
C	8.90554500	16.41170100	2.23321900
H	8.14156200	15.64507800	2.17108700
C	9.04017600	17.36755100	1.22744800
C	13.33451900	18.39109400	9.87476200
C	13.60739100	20.26708800	7.10240000
H	12.54300500	20.07243600	6.98508500
C	6.92141500	13.02348700	4.57732900
H	5.94531200	12.94647600	5.05417700
C	6.30201400	16.32371100	4.76173300
C	5.09642000	15.13208300	7.14388800
H	4.50237600	15.73114700	6.45912800
C	13.73440600	18.13372100	8.42347600
H	12.79629600	17.97635400	7.87168400
C	14.87943700	14.68453900	7.23199200
C	15.52698700	21.67781500	6.71922400
H	15.96587200	22.58039400	6.30239400
C	14.56038600	12.24738900	6.71131400
C	15.41432400	13.80611200	4.90669300
C	6.42565600	14.84469800	6.83762600
C	7.40420300	11.94746300	3.83569600
C	14.55277400	13.66430200	6.15087500
H	13.52252600	13.86839100	5.82743700
C	14.16547700	21.42467400	6.56716100
H	13.53598400	22.12945800	6.03019600
C	16.10945300	15.26082800	9.25861700
C	7.12261700	15.34075400	5.57823200
H	7.99590900	15.90986200	5.92439300
C	16.32401300	20.75757900	7.39690100
H	17.38972500	20.94029000	7.50970700
C	15.43777000	16.48116200	9.28126300
H	15.60566500	17.16351900	10.11307500
C	10.06676600	18.32059200	1.31809900
H	10.18672700	19.05995300	0.53539800
C	7.17641700	14.07726100	7.74044500
H	8.21799500	13.83772300	7.51619800
C	15.78667900	14.36386800	8.24260000
H	16.24682400	13.37753400	8.24168400
C	10.91620500	13.22051700	3.00203800
H	11.43785200	13.90956100	3.68375000
C	9.47574000	13.18301900	3.48709000
C	12.05380500	19.35514400	2.61891800
C	8.69637900	12.04042900	3.31763700
H	9.12311900	11.18202000	2.80111800
C	13.71211000	19.53043200	10.58504900
H	14.32195700	20.28952600	10.10393400
C	12.53996900	17.43587100	10.52241700
H	12.23369900	16.54490700	9.97910800
C	17.02117500	18.68604900	3.68158700
C	15.61255800	11.35646500	6.49741000
H	16.45016400	11.65266200	5.87116900
C	17.95785800	18.12500300	4.75956800
H	17.90068500	17.03321300	4.81832700
H	17.72212200	18.53669300	5.74765600
H	18.99247000	18.39278900	4.51642700
C	16.74496500	14.22348000	4.95664600
H	17.18291700	14.50761800	5.91025900
C	14.86825400	13.45992500	3.66805100
H	13.83542500	13.12311200	3.61969700
C	11.08803900	13.80819500	1.61415600
C	8.06173400	17.43523800	0.04631000
C	13.31479200	19.70856900	11.91189500
H	13.62312200	20.60273000	12.44764800
C	11.60575800	11.86783000	3.15235300
C	6.49093600	17.69404900	4.95943300
H	7.23950200	18.02642800	5.67634400
C	5.35103700	15.90781100	3.82743200
H	5.20306700	14.84621200	3.64737000
C	10.26844300	13.42956400	0.54938500
H	9.43898200	12.74922400	0.72757700
C	4.52067300	14.65937400	8.32528600
H	3.48200600	14.89193100	8.54644000
C	12.52816300	18.75272900	12.54472800
H	12.21583400	18.89291400	13.57606100
C	13.48258600	11.84119700	7.50625300
H	12.61814000	12.49536400	7.63229400
C	17.13233700	14.91534900	10.30795100
H	16.90118000	15.40080800	11.26146300
H	18.13399000	15.24819900	10.00647400
H	17.18301500	13.83446300	10.47212600
C	12.13829100	17.61268400	11.83979500
H	11.51594500	16.86115500	12.31844000
C	5.27050500	13.89938900	9.21613000
H	4.82397200	13.53464500	10.13739800
C	12.18709500	11.18544600	2.08285600
H	12.13799600	11.60630500	1.08285500
C	17.51314600	14.28573700	3.79554400
H	18.54816700	14.61335600	3.85185300
C	15.59976100	10.08847700	7.07986100
H	16.42803900	9.40711000	6.90235500
C	6.60445400	13.61302100	8.91817300
H	7.20328800	13.02455300	9.60887700
C	4.59775600	16.83934500	3.11713200

H	3.86242700	16.49766500	2.39304600
C	4.79223100	18.20351500	3.32245200
H	4.21195100	18.93012300	2.75991900
C	11.52504700	20.48454200	3.53867900
H	12.31830400	21.21657800	3.73092400
H	11.18990900	20.07734000	4.49812900
H	10.67868600	20.99241700	3.06159500
C	7.11765200	16.22709100	-0.00076700
H	6.47937600	16.17518500	0.88802300
H	7.67714500	15.28759400	-0.08010400
H	6.46414600	16.30958600	-0.87686100
C	11.69867500	11.31127100	4.43539700
H	11.26357300	11.83828600	5.28589300
C	15.62747100	13.53257900	2.50450300
H	15.17606600	13.26964500	1.55070700
C	5.74628900	18.62838600	4.24467600
H	5.91607000	19.69008300	4.40424600
C	16.95769300	13.94441600	2.56474000
H	17.55471700	14.00501200	1.65868500
C	12.50419800	19.97470700	1.29456400
H	11.67339900	20.50073300	0.81587000
H	12.88052500	19.21326700	0.60287400
H	13.29251300	20.71377400	1.46439700
C	7.20844100	18.71170300	0.18518300
H	6.48419700	18.77840700	-0.63676900
H	7.83571300	19.60930600	0.16450000
H	6.65719300	18.70223000	1.13245600
C	17.39761100	18.04357900	2.33166500
H	18.45546400	18.22577900	2.10246500
H	16.79381200	18.45642600	1.51645600
H	17.23189800	16.96061200	2.36387600
C	17.25880000	20.20559200	3.59721800
H	16.98026900	20.68956200	4.53929300
H	16.67781800	20.66627300	2.79248500
H	18.31914500	20.40822100	3.40231400
C	14.53278100	9.69696200	7.88308200
H	14.52088200	8.70860500	8.33518700
C	6.56735200	10.71527000	3.61499100
H	7.19202700	9.81890600	3.54686900
H	5.99701900	10.78792400	2.67985000
H	5.84732700	10.57479700	4.42719100
C	12.13520600	14.69880600	1.37061700
H	12.77092600	15.01330600	2.19593300
C	12.84452400	9.97077000	2.28451000
H	13.29418900	9.45747900	1.43827400
C	8.82654200	17.48719700	-1.28924500
H	9.44871900	16.59420100	-1.41014600
H	9.47518600	18.36603300	-1.35594500
H	8.11678100	17.53054200	-2.12454600
C	13.47092600	10.57872400	8.08828500
H	12.61948800	10.27621700	8.69315800
C	12.35318300	10.10201200	4.63463700
H	12.43087900	9.69591500	5.63934400
C	12.92938800	9.42358800	3.55996900
H	13.44577900	8.48091200	3.72107300
C	10.50288400	13.91453300	-0.73425600
H	9.85497300	13.61051500	-1.55255800
C	12.36973700	15.19187300	0.08990700
H	13.18601000	15.89005800	-0.07791200
C	11.55779300	14.79459100	-0.97003400
H	11.73761400	15.17794500	-1.97091900
Br	9.59865400	17.60376300	7.92728800

TS_Br_CaTHF

Final Single point energy: -7109.295752663728

Ca	0.24689600	3.55960300	4.33834000
Br	1.68777400	1.25835800	6.83887600
O	-0.32923200	5.77069600	3.85608000
O	-0.00890900	3.20189000	2.01848800
N	-1.92016700	4.09112300	5.05256300
N	2.10977100	4.96989500	4.15689200
C	-2.49865500	5.21641800	4.51648900
C	-1.66237500	6.14567100	3.85097700
C	3.40692300	7.48816200	6.31240600
C	1.94698100	6.16409800	3.51095800
C	-4.47752600	1.62730500	7.37688000
C	-2.77749000	3.36553100	7.22845100
C	-2.10678700	7.31381800	3.26698300
C	3.87096300	5.02442400	5.85662600
C	3.06181900	6.04411900	6.64513700
H	2.01784300	5.89902100	6.33726200
C	-2.76738300	3.26279800	5.81632500
C	2.96811800	6.97180500	2.97034000
H	3.98893100	6.62498100	3.08642800
C	-3.63634500	2.56415800	7.97706500
H	-3.63675400	2.65744900	9.06103400
C	-3.86830600	5.54965900	4.56355600
H	-4.53001200	4.86879000	5.08549700
C	-4.36705500	6.71646400	3.97954900
C	2.68467500	8.15720100	2.28885600
C	0.62316500	6.63186000	3.33103900
C	3.10893400	5.80540900	8.14990600
C	-2.28764600	5.77606200	7.80545600
C	0.29645200	7.81482700	2.70113600
C	4.15562200	3.65217700	3.86916200
C	3.38777900	4.58746200	4.59547900
C	4.70853400	7.89986500	6.02428600
H	5.50186500	7.15969400	5.95647300
C	4.34266400	4.01286700	1.36660400
C	5.05996100	4.50458000	6.35853500
H	5.40463900	4.82546600	7.34030900
C	2.39755600	8.45330700	6.36962400
H	1.37621300	8.14143300	6.57730700
C	-3.48334000	7.58449800	3.33234200
H	-3.85960000	8.48974600	2.86712700
C	-5.86164100	7.06202400	4.01704900
C	1.35307600	8.57441700	2.17441200
H	1.12173900	9.49682300	1.65150700
C	-1.15086300	8.28399100	2.57583300
C	-4.40397100	1.47566000	5.99503800
H	-5.01910600	0.71707900	5.51820900
C	4.00813400	6.46669600	8.99061900
H	4.69707700	7.19669500	8.57437500
C	-3.56457500	2.26790200	5.21169600
C	3.13601200	5.29089900	10.91262200
H	3.14219500	5.09533800	11.98161700
C	-1.81941600	4.33729900	7.90822700
H	-0.88225300	4.28456900	7.33469500

C	2.22013300	4.88666100	8.71650300
H	1.51732700	4.35742300	8.07608400
C	3.77075300	1.71101900	2.27734300
C	-3.60496300	6.13312500	8.09997700
H	-4.31605000	5.36170200	8.38718000
C	-1.47353700	3.91265600	9.33112200
C	5.33595700	3.14147300	4.41411600
H	5.88865600	2.38281900	3.86201100
C	4.02686600	6.20706800	10.35978100
H	4.73572700	6.73084000	10.99594600
C	-1.39019100	6.77475300	7.42713800
H	-0.36320900	6.50262100	7.18946600
C	5.72039300	4.23553200	1.30875400
H	6.35895300	3.87712700	2.11104100
C	3.69105200	3.21916900	2.48893800
H	2.62387000	3.48119100	2.44117600
C	-5.42790200	0.80235000	8.20296300
H	-4.97099200	0.50230000	9.15164500
H	-5.73852900	-0.09920500	7.66675500
H	-6.33393300	1.37220100	8.44519800
C	-1.73209000	4.70224400	10.45101200
H	-2.19695600	5.67617500	10.32972100
C	2.68085600	9.79848200	6.15925700
H	1.88021300	10.53258300	6.20132900
C	5.80756000	3.55574500	5.65590200
C	-0.85736600	2.66860700	9.52032500
H	-0.62533100	2.05198000	8.65467200
C	-6.40851500	7.10416900	2.57691200
H	-7.48169000	7.33184800	2.58367400
H	-6.26526700	6.13652200	2.08225600
H	-5.90165900	7.86830400	1.97859300
C	-0.52916600	2.21885800	10.79269400
H	-0.04684700	1.25218000	10.91330300
C	-3.43349100	2.00030000	3.71489900
H	-2.96904200	2.89850500	3.28499700
C	3.75066000	10.43955100	2.12484600
H	3.92594600	10.47036900	3.20508100
H	2.78774800	10.91957000	1.92279300
H	4.53214400	11.03013400	1.63085300
C	2.22957700	4.63186500	10.08417000
H	1.52023900	3.92231900	10.50098000
C	-1.52603500	8.38470200	1.08060800
H	-2.55568900	8.73839200	0.96283300
H	-1.44080400	7.40369500	0.59995700
H	-0.86179000	9.08344000	0.56166100
C	3.78437900	8.98785300	1.61296700
C	3.98888600	10.20289200	5.89609200
H	4.21550100	11.25358100	5.73641400
C	4.99921100	9.24758600	5.82335200
H	6.01971800	9.55099200	5.60390300
C	-3.11575700	8.44971500	7.62646100
H	-3.43996700	9.48382800	7.54611000
C	6.28603000	4.91601900	0.23321100
H	7.35989300	5.08199500	0.20691600
C	3.54588000	4.49907200	0.32749700
H	2.46934200	4.34830800	0.37136300
C	-1.39857800	4.25473300	11.73119400
H	-1.60804400	4.88649500	12.59045900
C	-0.80326400	3.01095400	11.90894200
H	-0.54418900	2.66316700	12.90531600
C	-6.06157600	8.44220100	4.67254100
H	-5.54304300	9.23132500	4.11902600
H	-5.67656500	8.43892600	5.69836100
H	-7.12860600	8.69485100	4.70391300
C	-1.79940500	8.10220400	7.33089800
H	-1.09093000	8.86573000	7.01940700
C	-4.01549200	7.46050100	8.01978100
H	-5.04495300	7.72168400	8.25093200
C	3.21321100	0.86793300	3.24693200
H	2.80749900	1.28716500	4.16727600
C	-1.28341500	9.67734800	3.22994600
H	-0.61646700	10.39779800	2.74618600
H	-1.02220000	9.62236000	4.29247200
H	-2.30827900	10.05138700	3.14409100
C	0.30103500	2.03452100	1.19954000
H	0.13761200	1.14555300	1.81370000
H	1.35633800	2.08158600	0.89830300
C	5.48250000	5.38786000	-0.80248000
H	5.92429800	5.92318900	-1.63858500
C	5.18588200	8.42192900	1.87194000
H	5.29290300	7.40869900	1.46880600
H	5.41775400	8.39481600	2.94282800
H	5.93128000	9.05729700	1.37995600
C	7.06040900	2.97060300	6.25137100
H	6.81765800	2.23224700	7.02579200
H	7.67493200	3.74440200	6.72358100
H	7.66275100	2.46747700	5.48936200
C	4.10653300	5.17900500	-0.75007300
H	3.46659100	5.55115900	-1.54586000
C	3.54361700	8.98944000	0.09017300
H	4.33116100	9.56027500	-0.41770300
H	2.57843800	9.44154700	-0.16077100
H	3.55408300	7.96559800	-0.30016400
C	-4.78718200	1.85013200	3.04503700
C	-2.45179300	0.85820600	3.44129000
C	-6.68220200	6.03753200	4.81075000
H	-7.73592600	6.33827500	4.81009700
H	-6.34969800	5.97642800	5.85342500
H	-6.61934500	5.03624100	4.36944100
C	-6.65517100	2.89939700	1.90102800
H	-7.10264400	3.78726000	1.46191900
C	3.18929400	-0.50979300	3.06981000
H	2.75070200	-1.14016700	3.83924200
C	4.30893700	1.13280000	1.12658100
H	4.74534300	1.76406000	0.35791400
C	-0.63875100	4.22783700	1.17788700
H	-0.06116000	5.15285100	1.27229500
H	-1.65320600	4.39120200	1.56274900
C	3.72737900	-1.07876300	1.91536600
H	3.71184900	-2.15621500	1.77541300
C	-1.41188500	0.57827400	4.33850600
H	-1.35652700	1.10808500	5.28844000
C	-0.63897700	3.66127000	-0.23741200
H	-1.51139300	3.99691500	-0.80417900
H	0.26448600	3.97134000	-0.77436700
C	4.28860700	-0.25142000	0.94808100
H	4.71546100	-0.68070800	0.04529300
C	-5.48802900	0.63909900	3.02035800

H	-5.03406600	-0.25613300	3.43741200
C	-5.38680600	2.97505000	2.47178200
H	-4.85342600	3.92377400	2.48768300
C	-7.34643500	1.69074000	1.89019000
H	-8.33496200	1.62788300	1.44364900
C	-6.75539500	0.55978400	2.45055000
H	-7.28222900	-0.39078400	2.44245600
C	-0.47425200	-0.41802600	4.06993300
H	0.32229700	-0.59810600	4.78668400
C	-0.62203100	2.14876400	0.00139800
H	-1.62299100	1.78568100	0.25824400
H	-0.25031700	1.58261300	-0.85710700
C	-2.51402100	0.11127300	2.26025300
H	-3.29964000	0.31309800	1.53814600
C	-0.56611000	-1.16986600	2.90206500
H	0.15763500	-1.95314000	2.69432800
C	-1.59091900	-0.89858500	1.99896500
H	-1.67014000	-1.46910800	1.07705000

TS_BrCa_THF

Final Single point energy: -7109.281679852495

Ca	4.98910900	9.09447200	13.06358600
Br	5.78305400	8.00107500	10.63264000
O	4.96041900	7.54542900	14.83888500
O	4.14661300	11.67453400	10.03032000
N	6.89909300	9.32571000	14.40466400
N	2.81676500	8.27866300	13.40563500
C	7.93362200	10.26632200	14.21664800
C	8.04446700	8.60015700	16.47659800
H	8.84064900	9.31168300	16.29354400
C	0.86451200	9.61895700	12.74471100
C	6.99605300	8.54358700	15.52767300
C	1.67628400	8.47232000	12.59585500
C	7.93404700	11.49234900	14.91907900
C	-0.33706800	9.72312700	12.04390000
H	-0.95678800	10.60565600	12.18786900
C	2.61797500	7.44261800	14.48123000
C	8.08008400	7.77652700	17.60023700
C	0.99676100	10.42480900	15.13067700
C	5.99284400	6.74198200	16.88125800
C	5.98487500	7.59393300	15.79126900
C	1.30634200	10.73810100	13.67983600
H	2.40374200	10.78852500	13.61021700
C	1.36416100	6.93840800	14.90153400
H	0.49470500	7.23820600	14.32982000
C	0.80432100	12.09885100	13.20988700
C	8.95784600	12.41480900	14.71257400
H	8.95349900	13.35015800	15.26719900
C	3.63838200	6.17191000	16.33585100
C	1.31563600	7.53136800	11.60150700
C	9.22034200	7.85139100	18.62586300
C	9.98742600	10.96486400	13.11763400
H	10.78615000	10.75635800	12.40842400
C	9.99887900	12.16896000	13.81814300
C	-0.75283300	8.74078900	11.14749100
C	8.97884300	10.01824000	13.29763600
C	1.22523700	6.09897400	16.00423600
C	1.12513200	12.50415000	11.90747100
H	1.69336500	11.83217300	11.26894000
C	-0.30876800	10.15184600	15.54729700
H	-1.11343800	10.14580100	14.81527300
C	0.11219700	7.67523900	10.91015800
H	-0.14402800	6.94628400	10.14335500
C	2.01914100	10.40630500	16.07837600
H	3.04159100	10.60510200	15.76499400
C	-0.14531200	5.58609800	16.47108900
C	3.72397200	7.03807100	15.25915600
C	2.37018300	5.71701200	16.71522900
H	2.27659400	5.04788500	17.56159600
C	2.29154000	6.13641900	9.74391200
C	7.04768500	6.85199000	17.79657300
H	7.07095500	6.19789600	18.65976900
C	6.78044900	11.81069700	15.86129600
H	6.39062600	10.84890300	16.21631300
C	9.46736900	7.55092700	13.41050300
C	0.09225500	12.97996400	14.02061300
H	-0.15473100	12.69787500	15.03958600
C	5.62116900	12.50114400	15.14901500
C	9.00075000	8.69998200	12.53711500
H	7.95812600	8.47607900	12.27730500
C	2.26009800	6.39082000	11.25021300
H	3.26636300	6.74193000	11.51897800
C	0.74142800	13.74887000	11.42834700
H	1.00745600	14.04315600	10.41621400
C	2.02399300	5.12241000	12.04785400
C	-0.29454600	14.23411900	13.54341500
H	-0.84609200	14.90768900	14.19421100
C	4.92858500	5.65425300	16.96468500
C	-0.58728800	9.89186300	16.88508600
H	-1.60901900	9.68573000	17.19344300
C	10.64657000	7.62977700	14.15470800
H	11.23187000	8.54660200	14.13309600
C	5.55601600	12.61442800	13.75682300
H	6.37087000	12.22840900	13.14728200
C	1.74875800	10.13267100	17.41684800
H	2.56090800	10.11468900	18.13904900
C	7.24955600	12.56327400	17.09529800
C	-1.28565400	6.04713100	15.55484100
H	-1.36747800	7.13972300	15.52993700
H	-2.23544600	5.64663700	15.92694100
H	-1.14613000	5.68814600	14.52836800
C	2.13164000	4.87176900	9.17718400
H	1.95274300	4.01212000	9.81588500
C	9.90459100	6.47527300	18.74513000
H	9.20183500	5.70098700	19.06829800
H	10.71877500	6.52210300	19.47880800
H	10.32462400	6.17139600	17.78029800
C	0.44189700	9.88102100	17.82587300
H	0.22669200	9.66782100	18.86948900
C	11.07313400	6.55200200	14.92489600
H	11.99494700	6.62749100	15.49610800
C	-0.42839300	6.10649200	17.89361700
H	0.33410200	5.76447600	18.60130000
H	-1.40410000	5.74545500	18.24268400
H	-0.43937000	7.20119400	17.90855100
C	0.02536600	14.62399500	12.24775000
H	-0.27451000	15.60062100	11.87761400
C	4.57002600	13.02990400	15.90744400

H	4.59258200	12.93257100	16.99032500
C	10.29332900	8.87791600	18.24030100
H	10.74694000	8.63762700	17.27207800
H	11.08677800	8.87427900	18.99598500
H	9.88553300	9.89344200	18.18723000
C	-2.07903300	8.84127600	10.44215400
H	-2.87008000	8.34741700	11.02106600
H	-2.04399400	8.35835200	9.46052400
H	-2.37823100	9.88508900	10.30507900
C	0.75476200	4.55013800	12.15860000
H	-0.10083000	5.05439900	11.71651400
C	11.08265900	13.18918500	13.59106200
H	10.80928200	13.88044200	12.78356200
H	12.02409400	12.71021600	13.30467600
H	11.25669800	13.78893900	14.48975900
C	4.48860500	13.27425600	13.14360600
H	4.45744200	13.35660900	12.06071100
C	8.64805500	8.24219400	20.00249300
H	8.14994100	9.21725600	19.95576300
H	9.45454800	8.30395300	20.74356400
H	7.91802700	7.50617700	20.35450300
C	2.53282300	7.21949900	8.88750900
H	2.66917100	8.20959200	9.31473900
C	9.73579600	8.80004800	11.20810800
C	3.51330500	13.69582900	15.29892700
H	2.71155200	14.10587300	15.90775700
C	3.47507400	13.83345500	13.91358200
H	2.65049600	14.35506800	13.43828700
C	10.86205100	8.04229500	10.88917100
H	11.26374300	7.34166700	11.61525100
C	-0.15049300	4.04569400	16.50020500
H	0.05846100	3.64146800	15.50490400
H	-1.13219200	3.67881000	16.82474300
H	0.60178600	3.65200200	17.19111400
C	8.71351100	6.37786600	13.46883100
H	7.78445200	6.31661000	12.90525700
C	11.47889200	8.16991500	9.64287100
H	12.35611000	7.56961500	9.41578400
C	0.57616000	3.34142900	12.82361900
H	-0.41823900	2.90866000	12.89872700
C	7.34906700	13.95730600	17.13268600
H	7.03344800	14.54213900	16.27204700
C	10.31357900	5.38424100	14.97716900
H	10.63951800	4.54648600	15.58783700
C	4.46686100	10.64489600	7.94249000
H	4.43775500	9.57532100	8.17075400
H	4.27211300	10.77893200	6.87435100
C	2.60042500	7.04617500	7.51166500
H	2.79126500	7.90228000	6.86935000
C	3.10797900	4.46497000	12.63079200
H	4.10058600	4.90482300	12.55307600
C	5.46782400	12.08111400	9.63260100
H	6.13660200	11.90904900	10.48291400
H	5.46324300	13.15689000	9.39544700
C	7.63561300	11.83644400	18.22354400
H	7.54948500	10.75210900	18.20221900
C	2.19662900	4.69381300	7.79346700
H	2.06543100	3.69906400	7.37541500
C	2.42807500	5.77776500	6.95467500
H	2.47840800	5.63950000	5.87806600
C	1.66562900	2.69075600	13.40119000
H	1.52529200	1.75100700	13.92859500
C	2.93263700	3.26004700	13.30774200
H	3.78770400	2.76632900	13.76147800
C	9.12801400	5.30228400	14.25062300
H	8.52202300	4.40101400	14.29534400
C	5.82232300	11.24427100	8.38734600
H	6.26934100	11.87273000	7.61144200
H	6.53014400	10.44910800	8.63656300
C	7.83826300	14.60469300	18.26424000
H	7.91060300	15.68910300	18.27459700
C	5.41763700	4.45644400	16.11003100
H	6.36508500	4.07089300	16.50497200
H	5.57468400	4.76234500	15.06995400
H	4.67043600	3.65463300	16.12452800
C	8.12574700	12.47964200	19.35712300
H	8.42011200	11.89430100	20.22465100
C	8.23183000	13.86853100	19.38037300
H	8.61108700	14.37477500	20.26383000
C	10.97530100	9.05387600	8.69533500
H	11.45417600	9.15069000	7.72477000
C	4.71375600	5.16988900	18.40181400
H	3.97706900	4.36284500	18.42937000
H	4.36856000	5.98181400	19.05095600
H	5.64030400	4.76173900	18.81415900
C	3.45050700	11.39009500	8.80816300
H	3.13792400	12.33366200	8.32908400
H	2.56004500	10.80472700	9.05969300
C	9.23327400	9.68248800	10.24181800
H	8.34740400	10.26990300	10.47287600
C	9.84264300	9.81062700	9.00080900
H	9.43115800	10.49840100	8.26632900

TS_F_A_BrPent

Final Single point energy: -2871.198363472650

F	0.34368600	-0.39449500	-2.48863200
C	1.00210000	-0.71360200	-4.56662000
H	0.03304200	-0.28401500	-4.76702500
H	1.75371100	-0.05451900	-4.16381500
C	1.12461700	-2.19256400	-4.37964300
H	0.45807200	-2.44028200	-3.54511300
H	0.74143500	-2.71638400	-5.26415900
C	2.54215800	-2.65637500	-4.06047200
H	2.89918500	-2.12022200	-3.16962800
H	3.21115300	-2.38083600	-4.88766600
C	2.62834900	-4.16213900	-3.81735500
H	2.25339400	-4.69292400	-4.70383000
H	1.95935900	-4.43363200	-2.98876500
C	4.04977100	-4.62602500	-3.50440000
H	4.09132700	-5.70638500	-3.32868400
H	4.72745400	-4.39337500	-4.33416300
H	4.43566100	-4.12398500	-2.60950900
Br	1.74902400	-0.39652800	-6.76897900

TS_F_axial2equitoral

Final Single point energy: -4762.917402241246

Ca	-0.75566500	-0.28429400	1.29749800
O	-0.19978400	1.36377400	-0.26247400

Cl	-1.82405500	-0.94287400	3.54361800
N	1.46115500	0.33577200	1.53929800
N	-2.15023200	-0.40398200	-0.54696500
C	2.24286600	0.02673000	2.66498200
C	3.37247200	1.49517300	0.46801200
H	4.05254900	1.04209600	1.18057900
C	1.14589000	1.74688500	-0.36426000
C	-0.95024300	1.45586100	-1.44406000
C	-2.92286900	-1.54611800	-0.82395600
C	2.00302200	1.17226100	0.59537900
C	3.84652600	2.33478900	-0.53872700
C	2.43301800	0.97101600	3.70559300
C	2.92875000	2.92472400	-1.42006900
H	3.28018200	3.60158700	-2.18901600
C	-0.64739200	2.39510300	-2.41312000
C	-4.23796400	-1.67929400	-0.32469200
C	2.62397900	3.46500000	3.12242200
C	1.55866000	2.64995300	-1.32729700
C	3.98076300	3.56988400	3.42935300
H	4.46877500	2.77543600	3.98744100
C	-1.96874100	0.49213300	-1.57069300
C	-2.72290400	0.54678400	-2.76456100
H	-3.51375900	-0.18476600	-2.88456400
C	-2.47254400	1.49275500	-3.75698900
C	1.09690200	2.67811000	4.96992700
C	2.02373000	4.49044300	2.38598500
H	0.96775700	4.41448000	2.13363500
C	-4.98187400	-2.82187900	-0.61807700
H	-5.99645200	-2.90457600	-0.23265400
C	-5.31092000	0.61469600	-0.28353000
C	-7.21223100	-0.75768300	1.45290300
H	-7.57051300	-0.09485500	0.67073900
C	1.75354400	2.33076300	3.63402200
H	0.93761300	2.21790100	2.90667600
C	2.76639400	-1.27498500	2.84528300
C	4.10845400	5.70053500	2.29643600
H	4.68436400	6.56461300	1.97622700
C	2.47215500	-3.73973500	2.34967800
C	3.49053300	-2.19477100	0.60556800
C	-5.85663000	-1.07893100	1.52339100
C	-4.45553300	-3.87011800	-1.37261700
C	2.53076500	-2.33068200	1.77498100
H	1.53229200	-2.14093000	1.35420300
C	2.75723800	5.59691700	1.97040800
H	2.27350300	6.37989000	1.39212000
C	3.74941800	-0.63847900	4.98187600
C	-4.81693900	-0.56293400	0.53474500
H	-3.98162100	-0.18216500	1.13823000
C	4.71711200	4.68057200	3.02302000
H	5.77338400	4.74575200	3.27150900
C	3.17604300	0.62283600	4.83339400
H	3.28408200	1.35020100	5.63681200
C	-1.42800700	2.41057600	-3.57482300
H	-1.22312400	3.15045000	-4.33899000
C	-5.42442600	-1.92576100	2.55203700
H	-4.36764800	-2.17392000	2.62357700
C	3.50992600	-1.58161400	3.98370300
H	3.90119700	-2.59055100	4.10078700
C	-0.89064600	-2.60134700	-1.92012100
H	-0.42547000	-1.86127200	-1.25001200
C	-2.35836300	-2.64098100	-1.52541900
C	0.48811700	3.37614600	-2.13901400
C	-3.12964500	-3.77079100	-1.79235900
H	-2.67364800	-4.60998700	-2.31621400
C	1.53048700	3.72090400	5.78909500
H	2.36347500	4.34413500	5.47618800
C	0.01528800	1.89841800	5.39655300
H	-0.33360400	1.07941900	4.77026800
C	5.34593800	2.59672100	-0.73618200
C	3.39703600	-4.73291100	2.03357800
H	4.21147900	-4.51475700	1.34865500
C	6.19570600	2.02499800	0.40593400
H	6.10538300	0.93554900	0.47169000
H	5.90877100	2.45486200	1.37231800
H	7.25059600	2.26222400	0.22714700
C	4.84683700	-1.92117800	0.79247200
H	5.22751000	-1.75656000	1.79761600
C	3.01742100	-2.38262700	-0.69396500
H	1.96270500	-2.59726100	-0.84922900
C	-0.61525000	-2.09137400	-3.32247300
C	-3.32993400	1.58322700	-5.02701200
C	0.90261100	3.97445700	7.00983800
H	1.25738200	4.78956700	7.63532000
C	-0.18711300	-3.92590200	-1.63336000
C	-5.00682300	1.91385000	0.12622000
H	-4.37708500	2.06090100	1.00148500
C	-6.10468300	0.43767600	-1.41874400
H	-6.33332600	-0.56946800	-1.76037500
C	-1.35793300	-2.51712800	-4.42439800
H	-2.20922200	-3.17678000	-4.27685300
C	-8.11660600	-1.27651500	2.38111600
H	-9.16886300	-1.01425700	2.30779400
C	-0.17119400	3.19397400	7.42472300
H	-0.66154300	3.39459600	8.37344900
C	1.42406700	-4.05483000	3.22364100
H	0.69370900	-3.28820800	3.47763900
C	4.58685000	-0.97640700	6.18632700
H	4.28506600	-0.38547300	7.05670200
H	5.64796700	-0.76620400	6.00010000
H	4.50479000	-2.03749800	6.44171000
C	-0.61535200	2.15291300	6.60829100
H	-1.45695400	1.53767200	6.91630300
C	-7.67756200	-2.12029600	3.39553500
H	-8.38145100	-2.52158100	4.11953700
C	0.54202200	-4.62541100	-2.59468700
H	0.59247700	-4.25053000	-3.61250800
C	5.71189000	-1.85263100	-0.29698800
H	6.76588100	-1.64199400	-0.13525200
C	3.28145400	-6.01227300	2.57972900
H	4.01134000	-6.77415500	2.31853400
C	-6.32189800	-2.44122800	3.47869300
H	-5.96296200	-3.09075800	4.27286600
C	-6.60666900	1.53573100	-2.11190400
H	-7.22917100	1.38163900	-2.98956300
C	-6.30307800	2.82896500	-1.69147700
H	-6.68961500	3.68650600	-2.23560200
C	-0.06436300	4.52569400	-1.25820200
H	0.74089900	5.22568300	-1.00532400

H	-0.48519700	4.13219600	-0.32740700
H	-0.85163300	5.06762900	-1.79512900
C	-4.31505200	0.41405700	-5.15113200
H	-5.03373000	0.40214500	-4.32509000
H	-3.79149500	-0.54899800	-5.16897700
H	-4.87894100	0.51241100	-6.08555000
C	-0.21815900	-4.42801900	-0.32565900
H	-0.78422100	-3.89729000	0.43863300
C	3.87540300	-2.30168100	-1.78694700
H	3.48258700	-2.44152000	-2.79121400
C	-5.49266900	3.01522200	-0.57372100
H	-5.23916800	4.01965700	-0.24507100
C	5.22992500	-2.04147800	-1.59071300
H	5.90422800	-1.97805700	-2.44048300
C	1.05302400	3.97761400	-3.42779100
H	0.27806600	4.52806700	-3.96799000
H	1.45731900	3.20233200	-4.08788000
H	1.84782400	4.69277300	-3.19843600
C	-4.13643700	2.89625900	-4.98864000
H	-4.76834700	2.98155800	-5.88171400
H	-3.47207000	3.76629100	-4.95501000
H	-4.78117700	2.92445600	-4.10349200
C	5.79142700	1.92688200	-2.05139600
H	6.86505700	2.08411600	-2.21476100
H	5.24883400	2.34015600	-2.90830300
H	5.60078300	0.84829800	-2.01446200
C	5.62536400	4.10849000	-0.82464300
H	5.28880700	4.61542800	0.08557500
H	5.11942800	4.56887600	-1.67877000
H	6.70190600	4.28284000	-0.94198600
C	2.23667700	-6.31592300	3.44546500
H	2.14428700	-7.31349700	3.86614300
C	-5.26765500	-5.10484300	-1.66183300
H	-5.06680200	-5.48513400	-2.66863200
H	-6.33926100	-4.90236500	-1.57552500
H	-5.02545600	-5.90984500	-0.95634500
C	0.46376200	-1.22938700	-3.53169200
H	1.03834100	-0.87508800	-2.67763900
C	1.22126900	-5.79827000	-2.25964700
H	1.78517100	-6.32693500	-3.02379900
C	-2.43729100	1.58541600	-6.28183300
H	-1.84873400	0.66394400	-6.33882100
H	-1.74428000	2.43224900	-6.28885800
H	-3.06029900	1.65458500	-7.18203300
C	1.30357600	-5.32795200	3.76514000
H	0.47862200	-5.55299600	4.43602300
C	0.46264400	-5.58958400	0.01279400
H	0.44649200	-5.94461300	1.03966300
C	1.18802300	-6.28257200	-0.95697700
H	1.72631600	-7.18866900	-0.69232800
C	-1.01920700	-2.10223800	-5.70979300
H	-1.60845200	-2.44101800	-6.55809300
C	0.80191000	-0.80720500	-4.81401400
H	1.63814700	-0.12697500	-4.95510400
C	0.06505800	-1.25044200	-5.91022000
H	0.32529400	-0.92299000	-6.91318200

TS_F_CaBr

Final Single point energy: -6976.882963837047

Ca	11.15445400	15.76541800	6.16219400
O	11.85497400	16.93628500	4.21742000
F	9.94288600	17.59402400	7.51516100
N	13.45146600	16.31496400	6.19024100
N	9.76660000	15.36870400	4.29333100
C	14.31506300	15.95360200	7.23576400
C	15.23449700	17.75270700	5.24423200
H	15.89734100	17.49019500	6.06032700
C	13.10524700	17.53523300	4.16446800
C	11.01848700	17.02508500	3.11525000
C	8.87680500	14.29143700	4.24283500
C	13.94385000	17.17837800	5.25080700
C	15.65831100	18.61414000	4.23134200
C	14.37295400	16.70817700	8.42914300
C	14.77785400	18.92280200	3.18887700
H	15.09196500	19.60274100	2.40416300
C	11.27504200	17.86501300	2.05024700
C	7.70374300	14.29474900	5.03731700
C	13.96399300	19.21093200	8.16806900
C	13.48514600	18.37617100	3.13738700
C	15.26147700	19.62699700	8.47349200
H	15.92690700	18.95856300	9.01425300
C	9.89738200	16.16080200	3.18701800
C	8.99221600	16.22890400	2.10621200
H	8.12085500	15.58574400	2.15278600
C	9.18259100	17.10429400	1.03587900
C	12.87548300	17.90507300	10.05296100
C	13.13268400	20.07716300	7.45393600
H	12.12380200	19.75577800	7.20300800
C	6.85559700	13.19039500	5.03401500
H	5.95917400	13.21059600	5.65126900
C	6.92278200	16.70195900	5.05172200
C	5.13767300	15.52969300	7.09516000
H	4.68189400	16.03703900	6.24975500
C	13.41394000	17.87318400	8.62666800
H	12.54593700	17.67382700	7.98277800
C	15.08475500	14.76780600	7.15633300
C	14.87345600	21.74659700	7.38198600
H	15.22811200	22.72689700	7.07477100
C	15.14293200	12.36781700	6.32150300
C	15.57171200	14.28482400	4.71631900
C	6.49805700	15.22044300	7.06742600
C	7.13414700	12.05024500	4.27698300
C	14.86406900	13.82779700	5.97670800
H	13.78758800	13.88761200	5.75564100
C	13.58308000	21.33360300	7.05776200
H	12.92540900	21.99011900	6.49397800
C	16.12516000	15.25909500	9.30521700
C	7.40484900	15.52684900	5.88332600
H	8.35533100	15.85707200	6.32310300
C	15.71164600	20.88733300	8.08959900
H	16.72456600	21.19624200	8.33553400
C	15.27344400	16.35392800	9.43493700
H	15.29375400	16.93712600	10.35452200
C	10.32969500	17.90503000	1.01253600
H	10.48955000	18.59048300	0.18689100
C	7.06093900	14.58450000	8.18052400
H	8.12289800	14.34363200	8.17218800
C	15.99093100	14.45938700	8.16913700

H	16.58422900	13.55040400	8.08949000
C	10.51841300	13.02723300	2.77618900
H	11.14966300	13.81316000	3.21186900
C	9.18939100	13.11733500	3.51305200
C	12.52996900	18.73219900	2.00062800
C	8.32035100	12.02614800	3.54593300
H	8.59332700	11.11762000	3.01064900
C	13.11001100	18.95200700	10.94357900
H	13.69862000	19.80819100	10.62663500
C	12.10035100	16.82076400	10.48538600
H	11.90624100	15.99888100	9.79803300
C	17.06366500	19.23389400	4.22540400
C	15.98191700	11.55174900	5.56229700
H	16.49337600	11.96050800	4.69606500
C	17.91824900	18.75553100	5.40561200
H	18.05493900	17.66807300	5.38567600
H	17.46772800	19.02930900	6.36614300
H	18.90839600	19.22250100	5.35173400
C	16.93261400	14.59774800	4.72753900
H	17.48193100	14.54818800	5.66521500
C	14.87408300	14.36506000	3.51105700
H	13.81078400	14.13079500	3.49393000
C	10.46004000	13.30459800	1.28367300
C	8.15193900	17.24654500	-0.09289300
C	12.59230700	18.91363700	12.23991300
H	12.78776500	19.73921500	12.91956900
C	11.22314300	11.70470100	3.06515100
C	7.44569200	17.97284300	5.30397800
H	8.22913200	18.07796100	6.05565400
C	5.94819000	16.55390000	4.06314100
H	5.55612300	15.56323700	3.84189500
C	9.37558900	12.93832000	0.48632500
H	8.48979100	12.51125400	0.94875000
C	4.35501400	15.20116400	8.20247900
H	3.29718000	15.45144800	8.20470800
C	11.82781200	17.83086000	12.66018500
H	11.42153300	17.80340100	13.66767500
C	14.48549000	11.80078300	7.42217600
H	13.81108700	12.41741900	8.01077100
C	17.13965600	14.93015500	10.36834700
H	16.83489900	15.32536200	11.34234000
H	18.11794900	15.36668000	10.12859700
H	17.28089000	13.84851200	10.46197700
C	11.58011900	16.78228700	11.77228100
H	10.97577400	15.93417700	12.08350100
C	4.92293300	14.56355700	9.30115900
H	4.31411600	14.31301400	10.16574800
C	11.25673600	10.64694000	2.15425300
H	10.78378600	10.75856000	1.18218500
C	17.58499600	14.97217400	3.55719100
H	18.64494900	15.21226400	3.58206800
C	16.16951700	10.20920500	5.89707700
H	16.82644100	9.59300900	5.28852400
C	6.28411200	14.25831700	9.28610800
H	6.74368200	13.76985400	10.14152600
C	5.47814500	17.66070600	3.35989400
H	4.71311600	17.53243200	2.59821800
C	5.99855100	18.92664000	3.61976500
H	5.64014100	19.78950100	3.06437700
C	12.12573800	20.21855100	2.13173400
H	13.00943800	20.86373800	2.07366500
H	11.63096600	20.39441800	3.09303100
H	11.43551300	20.50161700	1.32921700
C	7.02587000	16.20997700	0.01137900
H	6.46180600	16.32197800	0.94334500
H	7.41899100	15.18807000	-0.03387400
H	6.32748000	16.34393800	-0.82281700
C	11.85414700	11.53927800	4.30312100
H	11.83243900	12.35066100	5.02892600
C	15.51882700	14.75434900	2.33927800
H	14.95644000	14.82549900	1.41148500
C	6.99156000	19.07673300	4.58659300
H	7.41518100	20.05862900	4.78290200
C	16.87856200	15.05563700	2.35800100
H	17.38358400	15.36161200	1.44563000
C	13.23937800	18.51749900	0.64573700
H	12.58081600	18.78377100	-0.18615500
H	13.53137000	17.46738600	0.53269000
H	14.13745300	19.13719200	0.56984500
C	7.52227800	18.65164700	-0.01992000
H	6.77558500	18.77760000	-0.81448300
H	8.28142600	19.43262000	-0.13595000
H	7.02774800	18.79890900	0.94654000
C	17.79754700	18.85602200	2.92393800
H	18.80489000	19.29104800	2.91961400
H	17.26569800	19.22413800	2.04073600
H	17.88952100	17.76837100	2.83494300
C	16.95080900	20.76837500	4.30295100
H	16.43670600	21.06913700	5.22181800
H	16.38977700	21.16999100	3.45277900
H	17.94902000	21.22486000	4.29884900
C	15.51957100	9.66056500	6.99675600
H	15.66421300	8.61529900	7.25659900
C	6.18665000	10.87993500	4.26318300
H	6.70638500	9.95377900	3.99866100
H	5.38431800	11.02762400	3.52848500
H	5.71042400	10.74235300	5.23945400
C	11.57847900	13.87595400	0.66828600
H	12.42394800	14.17850100	1.28352600
C	11.89796500	9.45050200	2.47503500
H	11.91183200	8.63869700	1.75217400
C	8.83135000	17.07462400	-1.46408000
H	9.31043300	16.09248300	-1.53486400
H	9.59554200	17.83866400	-1.63804000
H	8.08659300	17.15566200	-2.26578400
C	14.67155100	10.46602700	7.75863200
H	14.14523600	10.04923200	8.61363200
C	12.50056500	10.35062400	4.62326400
H	12.99680700	10.25143400	5.58478000
C	12.52416500	9.29810400	3.70861400
H	13.03272200	8.36997600	3.95613500
C	9.41510100	13.12063600	-0.89489100
H	8.56019600	12.82995200	-1.50027100
C	11.61906900	14.06760700	-0.70837900
H	12.49397900	14.52342900	-1.16491000
C	10.53800700	13.67951400	-1.49894500
H	10.56561800	13.82667600	-2.57530900
Br	10.99459700	13.47504000	7.82532000

TS_F_CaBr_

Final Single point energy: -6976.849632904292

Ca	11.22780200	15.65668400	6.10127200
O	11.83916600	16.96665300	4.24267100
F	9.91275800	18.57564900	7.67334500
N	13.45401300	16.29616300	6.17877000
N	9.76479800	15.37660900	4.31302200
C	14.30764600	15.94129600	7.23643500
C	15.26198200	17.68219400	5.19731400
H	15.93321900	17.40179400	6.00042600
C	13.10754700	17.52885800	4.16334400
C	10.99784800	17.05527700	3.14234000
C	8.89158200	14.28388400	4.23823400
C	13.95712000	17.14607400	5.22850900
C	15.68622100	18.53744000	4.17905300
C	14.34626800	16.70425000	8.42672200
C	14.79077600	18.87790700	3.15922300
H	15.10514900	19.55859800	2.37576500
C	11.24854800	17.90358300	2.08228300
C	7.72350000	14.24322400	5.03844700
C	13.81002000	19.17357200	8.04144400
C	13.48176900	18.37155300	3.13589500
C	15.11776000	19.63742300	8.19012400
H	15.85671700	19.01201500	8.68621000
C	9.88561600	16.18378800	3.21090200
C	8.97808500	16.24996100	2.13461400
H	8.11474500	15.59638400	2.17616500
C	9.15794300	17.13487600	1.07064400
C	12.89865900	17.95382500	10.06587200
C	12.87271300	19.97463000	7.38234400
H	11.84836200	19.60744000	7.27947100
C	6.88861600	13.12996300	4.99232000
H	5.99268400	13.11423900	5.60960300
C	7.02988300	16.67649600	5.17637200
C	5.10344000	15.46054500	7.05383400
H	4.71747600	16.05889400	6.23388600
C	13.35470000	17.84492500	8.61565600
H	12.45573900	17.57967200	8.04280900
C	15.07779000	14.75727300	7.17269700
C	14.54906200	21.68267100	7.03996300
H	14.83783000	22.65385500	6.64620100
C	15.09358800	12.33918100	6.39266000
C	15.57746200	14.21206000	4.74638700
C	6.44613200	15.08199500	7.06504200
C	7.18048600	12.02149000	4.19350900
C	14.85268500	13.79636000	6.01092400
H	13.77963700	13.86711800	5.77557100
C	13.24532800	21.21753100	6.87592200
H	12.51249400	21.82794200	6.35362700
C	16.11887600	15.28405000	9.31098100
C	7.42382100	15.43062400	5.94921400
H	8.36516300	15.67937900	6.45998400
C	15.48346100	20.88971200	7.70325000
H	16.50453900	21.24128900	7.82937900
C	15.25478400	16.37204200	9.43147900
H	15.27454600	16.96691500	10.34313100
C	10.29894000	17.94433500	1.04952100
H	10.44841700	18.63789200	0.22910100
C	6.91831200	14.32789300	8.14595400
H	7.96624500	14.03330000	8.16809600
C	15.98632800	14.46551000	8.18931900
H	16.58266200	13.55747800	8.12206900
C	10.55609000	13.08533000	2.74287700
H	11.16454100	13.88821500	3.18195000
C	9.22126700	13.14016200	3.47084700
C	12.49002200	18.79167000	2.05310700
C	8.36814700	12.03579800	3.46585400
H	8.65783000	11.14851900	2.90403400
C	13.33461300	18.95645500	10.93247900
H	14.01290500	19.72389200	10.57004500
C	12.00791300	16.99027500	10.55425300
H	11.65187900	16.20612800	9.88793200
C	17.10748400	19.11947000	4.14456200
C	15.90917100	11.48271800	5.65341300
H	16.43525700	11.85809200	4.78079000
C	17.96701400	18.62904800	5.31621900
H	18.07602200	17.53837300	5.30332100
H	17.53755500	18.92119500	6.28095900
H	18.96771100	19.07018400	5.24422400
C	16.94536600	14.49255400	4.75941900
H	17.48961800	14.44457900	5.70010600
C	14.88650000	14.29085700	3.53703400
H	13.81800700	14.08035200	3.51762900
C	10.50469600	13.36741500	1.25160400
C	8.12245300	17.27596600	-0.05340900
C	12.90359300	18.98872100	12.25911900
H	13.25555900	19.77802900	12.91843500
C	11.29408400	11.78395600	3.04993300
C	7.58810500	17.90998800	5.52175100
H	8.33919400	17.97908300	6.31472800
C	6.08960100	16.62020100	4.14555500
H	5.66760400	15.65948500	3.85688500
C	9.43983000	12.97518400	0.44037200
H	8.56259500	12.51645200	0.88799900
C	4.24928500	15.08481000	8.09118500
H	3.20668600	15.39103500	8.06422600
C	12.02345500	18.02265000	12.73608300
H	11.68260400	18.05139500	13.76750200
C	14.41476100	11.81716600	7.50235400
H	13.75953000	12.46763700	8.07641700
C	17.14177200	14.98346600	10.37419200
H	16.81267700	15.34350100	11.35396700
H	18.09812800	15.47349100	10.14988400
H	17.33564800	13.90853600	10.44655200
C	11.57336900	17.02217900	11.87390500
H	10.87600300	16.26804200	12.22924600
C	4.72674000	14.32954200	9.15761000
H	4.06192500	14.04160400	9.96754600
C	11.54928700	10.80435800	2.08979800
H	11.21724800	10.95357500	1.06618600
C	17.61113000	14.83395900	3.58653600
H	18.67626000	15.04965500	3.61259400
C	16.05173800	10.14189100	6.01562000
H	16.69042200	9.49253600	5.42230000
C	6.07008600	13.95453700	9.18202400
H	6.45969000	13.37360400	10.01404900
C	5.69087500	17.77973200	3.48481200

H	4.95177800	17.72192500	2.68962200
C	6.25177500	19.00739800	3.82921900
H	5.95265300	19.91158600	3.30519900
C	12.06339900	20.25534400	2.31369400
H	12.93629600	20.91772900	2.29695100
H	11.58111400	20.34193500	3.29333600
H	11.35486800	20.58921600	1.54718700
C	7.00582700	16.22873700	0.04792600
H	6.44342600	16.32892300	0.98225600
H	7.40773100	15.21053400	-0.00597900
H	6.30366900	16.36216400	-0.78305900
C	11.74097900	11.56734000	4.35928300
H	11.53892500	12.31502500	5.12554400
C	15.54536900	14.64699100	2.36260900
H	14.98959100	14.71769300	1.43094300
C	7.20718000	19.06536600	4.84275200
H	7.66000100	20.01677000	5.11140000
C	16.91181300	14.91561000	2.38317700
H	17.42762300	15.19551200	1.46853100
C	13.15839100	18.69760300	0.66627800
H	12.46898700	19.01136700	-0.12236400
H	13.47174000	17.66756900	0.46271600
H	14.03744500	19.34545300	0.60883800
C	7.48160000	18.67543700	0.03105000
H	6.73062400	18.79969200	-0.75960700
H	8.23370000	19.46334700	-0.08378300
H	6.99045100	18.81357400	1.00054700
C	17.80760600	18.70743800	2.83509700
H	18.82494500	19.11757000	2.80616500
H	17.26719200	19.07762800	1.95784800
H	17.87109700	17.61681900	2.75899300
C	17.04007600	20.65762900	4.20653000
H	16.54156400	20.98397900	5.12482600
H	16.48559600	21.06761200	3.35617500
H	18.05156000	21.08320000	4.18972000
C	15.37981000	9.63678000	7.12286900
H	15.48935400	8.59270800	7.40378000
C	6.24578500	10.84242800	4.13756600
H	6.77390200	9.93382000	3.83221900
H	5.43769200	11.01185300	3.41408300
H	5.77687600	10.66021700	5.11001500
C	11.61127200	13.97725000	0.65206600
H	12.44039100	14.30129500	1.27856600
C	12.23406500	9.63623800	2.42915700
H	12.42270800	8.88496600	1.66642900
C	8.79904300	17.11752200	-1.42749200
H	9.28580100	16.13962400	-1.50495200
H	9.55641800	17.88873900	-1.59961500
H	8.05117600	17.19703000	-2.22635400
C	14.55604600	10.48411200	7.86578600
H	14.01467900	10.10158100	8.72735800
C	12.42994600	10.40975800	4.69867700
H	12.78565200	10.27388800	5.71630200
C	12.67988600	9.43575100	3.73137900
H	13.22317700	8.53190600	3.99429400
C	9.48684900	13.17260500	-0.93864700
H	8.64632200	12.86320600	-1.55473600
C	11.66039400	14.18120000	-0.72257900
H	12.52602200	14.66634500	-1.16632400
C	10.59863000	13.76920000	-1.52687200
H	10.63180300	13.92735200	-2.60151300
Br	10.91432400	13.61270500	7.98040500

TS_FCa_Br

Final Single point energy: -6976.890619463749

Ca	11.09130000	15.87187500	6.21458600
O	11.80478700	17.03094500	4.27535900
F	10.10149200	17.26453400	7.42759100
N	13.43656200	16.29751600	6.19977100
N	9.72444300	15.43305000	4.32146700
C	14.30745600	15.93972700	7.24108000
C	15.25322000	17.66153200	5.21101200
H	15.92616700	17.36141800	6.00561300
C	13.08742000	17.55602000	4.19259900
C	10.97771600	17.10761300	3.16446600
C	8.86808200	14.33143300	4.24069500
C	13.93778300	17.14480500	5.25004100
C	15.68780400	18.51559600	4.19756400
C	14.38929200	16.71894000	8.41781600
C	14.79301600	18.88105000	3.18525800
H	15.11580200	19.56063900	2.40445600
C	11.24283800	17.94833500	2.10162300
C	7.68401100	14.28425500	5.01676300
C	13.97920100	19.20728100	8.07079300
C	13.47470300	18.39762100	3.16807200
C	15.26642100	19.65503700	8.37541200
H	15.92598000	19.02809200	8.97049000
C	9.86478100	16.23162200	3.22149500
C	8.97335200	16.29379500	2.12824500
H	8.10980600	15.63913400	2.16039700
C	9.16870800	17.17253600	1.06235100
C	12.93350400	17.98042400	10.03634200
C	13.15627500	20.01730600	7.28550100
H	12.15713900	19.66916200	7.03063600
C	6.87179000	13.15336700	4.98574100
H	5.96657500	13.13594900	5.59008400
C	6.79984800	16.65062400	5.03866300
C	5.07328700	15.46899900	7.10706700
H	4.61470600	16.02468000	6.29416800
C	13.43843000	17.89294900	8.60037000
H	12.55543900	17.66811800	7.98682100
C	15.06716100	14.74745000	7.17583600
C	14.88194400	21.69753700	7.14486500
H	15.23396500	22.66017100	6.78361900
C	15.08698900	12.32893400	6.39552700
C	15.53888900	14.20259900	4.74677600
C	6.42769900	15.14044600	7.04562500
C	7.19777300	12.03306400	4.21871800
C	14.82756900	13.78471900	6.01844200
H	13.75155500	13.85431400	5.79768600
C	13.60353200	21.25079500	6.81924100
H	12.95244800	21.86286100	6.20044500
C	16.14633700	15.27916200	9.29662700
C	7.32752300	15.49562000	5.86976000
H	8.26216500	15.86131400	6.31496600
C	15.71297700	20.89324300	7.92254400
H	16.71756500	21.22774800	8.16918300
C	15.30377400	16.38264000	9.41630000

H	15.34272600	16.98600600	10.32217600
C	10.30972200	17.98313700	1.05270200
H	10.46885700	18.67392800	0.23203300
C	6.99439200	14.43892200	8.11725300
H	8.05154500	14.17779000	8.08428200
C	15.98769400	14.45565600	8.18122600
H	16.57374100	13.54115600	8.11173900
C	10.56758000	13.13491000	2.78057700
H	11.16561800	13.94338700	3.22404100
C	9.22666500	13.17827800	3.49817800
C	12.48313300	18.83993600	2.09275700
C	8.39419300	12.05875600	3.50452400
H	8.70838100	11.16663200	2.96373700
C	13.14380600	19.08307700	10.86364200
H	13.69595500	19.94042400	10.48971600
C	12.20396900	16.89584200	10.54234400
H	12.03050600	16.02906000	9.90708500
C	17.12038900	19.06912500	4.15925300
C	15.88928600	11.47577200	5.63771900
H	16.39136000	11.85149700	4.75127600
C	17.98024600	18.54575300	5.31643200
H	18.06679400	17.45341000	5.28875000
H	17.56559400	18.83425900	6.28891100
H	18.98902900	18.96765300	5.24102600
C	16.91031800	14.46640500	4.74254300
H	17.46610600	14.40810700	5.67593500
C	14.83388300	14.29331900	3.54669700
H	13.76262700	14.09774300	3.54286700
C	10.51678600	13.41304900	1.28845400
C	8.14660200	17.31006100	-0.07473100
C	12.64916000	19.09906900	12.16948600
H	12.82602600	19.96766800	12.79872000
C	11.31285600	11.83836400	3.09015900
C	7.26034200	17.94443100	5.29241800
H	8.03003100	18.09088400	6.04834000
C	5.83836400	16.46073700	4.04412400
H	5.49195900	15.45358600	3.82202700
C	9.46291800	12.99441300	0.47570800
H	8.59503500	12.51801600	0.92324400
C	4.29914900	15.09597600	8.20689700
H	3.24550400	15.36184400	8.23567200
C	11.93087300	18.01562600	12.66287800
H	11.54277000	18.02975900	13.67775500
C	14.44013600	11.80400900	7.52234400
H	13.78867500	12.44725200	8.10811300
C	17.17626600	14.96726000	10.35002700
H	16.88204800	15.37157700	11.32357800
H	18.14900700	15.40644100	10.09310000
H	17.32430200	13.88751700	10.45367700
C	11.70657100	16.91118300	11.83870700
H	11.13912700	16.06065300	12.20739500
C	4.87001200	14.39346100	9.26316000
H	4.26783600	14.10695100	10.12121100
C	11.58587600	10.86386000	2.12956300
H	11.26883000	11.01582900	1.10161900
C	17.56604400	14.79981800	3.56186100
H	18.63435400	15.00068000	3.57468800
C	16.04913400	10.13634800	5.99799100
H	16.67667900	9.49013500	5.38946100
C	6.22617900	14.06810400	9.21414600
H	6.68858300	13.52749500	10.03606900
C	5.32448000	17.54508600	3.33714400
H	4.57130900	17.38221600	2.57036000
C	5.78478600	18.83352100	3.60020800
H	5.39192800	19.67928600	3.04206300
C	12.05258600	20.29661800	2.38507600
H	12.92479100	20.96039900	2.38566500
H	11.56766100	20.36075200	3.36526600
H	11.34500000	20.64593600	1.62441600
C	7.04376500	16.24612200	0.00073200
H	6.46571100	16.33179500	0.92683200
H	7.46137600	15.23431000	-0.05366000
H	6.35260000	16.37584700	-0.84009600
C	11.74067900	11.61822700	4.40524900
H	11.52657900	12.36255100	5.17111000
C	15.48276400	14.64187000	2.36423900
H	14.91691500	14.72024800	1.43920100
C	6.76229200	19.02853700	4.57428600
H	7.13952600	20.02810200	4.77478400
C	16.85296300	14.89128400	2.36725900
H	17.36108700	15.16370700	1.44604600
C	13.15358900	18.78189100	0.70534100
H	12.46392600	19.10891800	-0.07744300
H	13.47513000	17.75923400	0.47877000
H	14.02770300	19.43740000	0.66271600
C	7.48398800	18.69879800	0.01870100
H	6.74248400	18.82402200	-0.78083800
H	8.22662700	19.49866100	-0.07324300
H	6.97641400	18.81508100	0.98282900
C	17.80160100	18.66295100	2.83814900
H	18.82686900	19.05280200	2.80664600
H	17.26173100	19.05704300	1.97108500
H	17.84211200	17.57256000	2.74530200
C	17.08392900	20.60686700	4.24533100
H	16.60225100	20.92609800	5.17503700
H	16.52709800	21.04085700	3.40841400
H	18.10306800	21.01368600	4.22365300
C	15.40746600	9.62834100	7.12184000
H	15.52971400	8.58512600	7.40091900
C	6.29077400	10.83178600	4.17669400
H	6.85220400	9.92064300	3.94729100
H	5.51855800	10.94406000	3.40437300
H	5.77592300	10.68923300	5.13224800
C	11.61112900	14.04366500	0.68858100
H	12.42985000	14.39099600	1.31572100
C	12.26749000	9.69536000	2.47459400
H	12.46997900	8.94791000	1.71156500
C	8.84108600	17.17816000	-1.44261100
H	9.34719200	16.21047900	-1.52504900
H	9.58526300	17.96520900	-1.59984800
H	8.10023700	17.25158300	-2.24857400
C	14.59732900	10.47212400	7.88331400
H	14.07621300	10.08788000	8.75664000
C	12.42338200	10.45879000	4.75051000
H	12.76017700	10.31837700	5.77394100
C	12.69022900	9.48885700	3.78351200
H	13.22898500	8.58386800	4.05199100
C	9.50908400	13.18651300	-0.90400400

H	8.67725400	12.85565000	-1.52081700
C	11.65998800	14.24195200	-0.68695200
H	12.51633900	14.74356700	-1.13052700
C	10.60942000	13.80398100	-1.49230500
H	10.64241700	13.95740600	-2.56765900
Br	10.84946600	13.04788300	8.17355500

TS_FCaTHF_A_Brbiphen

Final Single point energy: -7711.037195033453

Ca	0.18290400	0.30557700	-0.81682200
F	0.81874600	-0.39835600	-2.76830200
O	0.01730900	-1.61607800	0.54346400
O	0.12335300	2.52093200	-1.62052200
N	1.91872300	0.25990300	0.85435200
N	-2.06923400	-0.31338300	-0.48376500
C	3.04772900	1.10651700	0.89251000
C	3.05899000	-1.19528300	2.51108300
H	3.86526900	-0.47687000	2.60219200
C	-3.76874200	1.44194400	-0.58378700
C	2.01253600	-0.88611100	1.60677300
C	-3.17455000	0.27556900	-1.11621600
C	3.22908400	2.09824700	1.88815800
C	-4.90979000	1.97694100	-1.17799000
H	-5.36489700	2.86702900	-0.74758000
C	-2.32760800	-1.43720300	0.25709800
C	3.08151500	-2.37207200	3.25906800
C	-3.41728700	1.33163200	1.91286900
C	0.99631600	-3.05830700	2.20765800
C	1.01104000	-1.87629200	1.48965000
C	-3.12456500	2.09302700	0.63477600
H	-2.03865200	2.00739500	0.48112700
C	-3.61039600	-1.95038300	0.56560800
H	-4.46503400	-1.40612500	0.18142100
C	-3.41475900	3.58650700	0.70804300
C	4.38687700	2.87928400	1.88478600
H	4.53795700	3.60228500	2.68365800
C	-1.37384800	-3.31980800	1.53801500
C	-3.67868000	-0.23608000	-2.33386800
C	4.21123900	-2.68160100	4.25140500
C	5.16347900	1.81164300	-0.10079800
H	5.90473700	1.70606600	-0.89176800
C	5.36206400	2.76322500	0.89710700
C	-5.46973900	1.41618100	-2.32745500
C	4.04707000	0.97791900	-0.10440300
C	-3.79166600	-3.08677800	1.35183200
C	-2.95469100	4.39259500	-0.34185700
H	-2.42824500	3.92636500	-1.17245400
C	-4.72835100	1.07955600	2.32455500
H	-5.55768600	1.41394700	1.70467300
C	-4.81321900	0.33450200	-2.91208200
H	-5.17640800	-0.05577800	-3.86180700
C	-2.36650500	0.86125400	2.69986300
H	-1.34249700	1.01861800	2.36766800
C	-5.19013900	-3.58984200	1.73822900
C	-1.24582200	-2.15440800	0.80504500
C	-2.66535700	-3.77901900	1.82293300
H	-2.79363600	-4.67631300	2.41626500
C	-2.78067100	-1.07577200	-4.53037000
C	2.03687000	-3.29430400	3.11413900
H	2.04056700	-4.21030400	3.69281400
C	2.17277400	2.32205000	2.96270000
H	1.51003400	1.44946400	2.93658500
C	4.48822300	-1.43849800	-0.68228600
C	-4.09336200	4.19746000	1.76073900
H	-4.44787900	3.60030600	2.59537700
C	1.29366800	3.54604200	2.71946000
C	3.91873000	-0.11272500	-1.15614300
H	2.84613500	-0.29270400	-1.29550200
C	-2.92452100	-1.35396700	-3.03697000
H	-1.90553500	-1.32061400	-2.62446000
C	-3.17041700	5.76433100	-0.34273200
H	-2.80198600	6.36890200	-1.16755900
C	-3.43861800	-2.75044000	-2.73928500
C	-4.31618800	5.57573400	1.76208000
H	-4.84751600	6.03079400	2.59399800
C	-0.09484300	-4.07749200	1.88553200
C	-4.98057900	0.40448700	3.51516800
H	-6.00625000	0.22046900	3.82438100
C	5.77156900	-1.53870200	-0.13944800
H	6.37512500	-0.64245800	-0.01713000
C	1.72371700	4.68435000	2.03614300
H	2.70959900	4.70265300	1.58108600
C	-2.61207900	0.17248400	3.88456900
H	-1.77870700	-0.19653300	4.47714400
C	2.77088700	2.38589000	4.36630200
C	-6.30833400	-2.75839200	1.09686500
H	-6.27076400	-1.71257200	1.42264600
H	-7.28086800	-3.16828500	1.39209500
H	-6.24903500	-2.78215000	0.00236400
C	-3.09594400	-2.00709000	-5.51952500
H	-3.50235100	-2.97493500	-5.24073900
C	4.84907600	-4.04375100	3.91642500
H	4.12010800	-4.85815300	3.97139900
H	5.65679900	-4.26396400	4.62524600
H	5.26933000	-4.03121200	2.90506500
C	-3.92244900	-0.04941500	4.30125000
H	-4.11870500	-0.58668100	5.22516300
C	6.28314700	-2.77321600	0.24994100
H	7.28391100	-2.83403600	0.66980200
C	-5.35082400	-3.51079800	3.26928900
H	-4.61013100	-4.13474300	3.78022800
H	-6.34975300	-3.85554900	3.56470800
H	-5.22279800	-2.47964200	3.61468000
C	-3.85817900	6.36450100	0.71314500
H	-4.03001600	7.43742100	0.71614500
C	0.01242600	3.55367800	3.28120400
H	-0.33104900	2.67991700	3.83056300
C	5.32428600	-1.62629000	4.22570100
H	5.78492800	-1.55640800	3.23326100
H	6.10509500	-1.90608700	4.94190300
H	4.95363500	-0.63439300	4.50483500
C	-6.73072600	1.97841800	-2.92780700
H	-7.61947100	1.50719700	-2.48865800
H	-6.76829700	1.80275900	-4.00741500
H	-6.81091900	3.05515200	-2.74818600
C	-4.78550200	-3.09152100	-2.88042200
H	-5.50897800	-2.32888200	-3.15724300
C	6.57400200	3.65601800	0.89016600

H	6.80176600	4.02232600	1.89582600
H	6.41368400	4.53244100	0.24921400
H	7.45299400	3.12934100	0.50517400
C	0.89391200	5.79826000	1.91383300
H	1.24754100	6.67298600	1.37400500
C	3.62759600	-2.74305100	5.67649500
H	3.14197700	-1.79677900	5.93853700
H	4.42332200	-2.93587100	6.40682300
H	2.88181100	-3.53961300	5.76598400
C	-2.24480700	0.15768700	-4.92597400
H	-1.99285400	0.89298900	-4.16479300
C	4.43318500	0.33028800	-2.51785100
C	-0.81973600	4.66079500	3.15851600
H	-1.81552700	4.63923500	3.59172300
C	-0.38077900	5.79201300	2.47221800
H	-1.03192500	6.65568000	2.36916900
C	5.46807200	-0.30527500	-3.20155700
H	5.97332900	-1.15338100	-2.74813200
C	-5.37287400	-5.05371800	1.29546200
H	-5.27620200	-5.14243200	0.20853600
H	-6.36864100	-5.41221300	1.58474000
H	-4.63084400	-5.71239500	1.75779100
C	3.72229200	-2.59828900	-0.80624200
H	2.71419400	-2.53270900	-1.20921700
C	5.84933200	0.12405500	-4.47480200
H	6.65342500	-0.38996100	-4.99470600
C	-5.21108600	-4.40090600	-2.67398000
H	-6.26304900	-4.64989300	-2.78792300
C	3.20990900	3.58837800	4.93032900
H	3.09559600	4.51694500	4.37693400
C	5.51482800	-3.92791300	0.10783000
H	5.91327700	-4.89157000	0.41356900
C	0.88315900	4.22026200	-3.07838000
H	1.94753100	3.98626400	-3.19461600
H	0.57542200	4.86350300	-3.90708000
C	-2.02996000	0.45023800	-6.26627600
H	-1.60101000	1.40838500	-6.54810200
C	-2.53281200	-3.74539400	-2.36651600
H	-1.48589000	-3.48594900	-2.22820800
C	0.59606300	3.62725300	-0.78974500
H	1.59811600	3.37122000	-0.42229300
H	-0.08461300	3.72982300	0.06183700
C	2.88727600	1.21584100	5.12178700
H	2.53963300	0.27661000	4.69653900
C	-2.88553800	-1.71370900	-6.86870700
H	-3.13583400	-2.45543700	-7.62260300
C	-2.35248000	-0.48774100	-7.24833000
H	-2.17866500	-0.26421800	-8.29703800
C	-4.29551800	-5.39024900	-2.31986000
H	-4.62939200	-6.41161300	-2.15779900
C	-2.95338100	-5.05579000	-2.15775000
H	-2.23235600	-5.81414100	-1.86269700
C	4.22865400	-3.83539600	-0.41691800
H	3.61495100	-4.72668600	-0.52418600
C	0.61909900	4.84403400	-1.70360600
H	-0.35260600	5.35028200	-1.69110100
H	1.38799700	5.56027400	-1.40323500
C	3.77576700	3.61605100	6.20213600
H	4.11286600	4.56106100	6.62000200
C	0.34288400	-4.85834500	0.61824700
H	1.27695400	-5.39981700	0.80966000
H	0.50311200	-4.17769100	-0.22542000
H	-0.43374100	-5.58005400	0.33810100
C	3.44683300	1.24219200	6.39714900
H	3.52704600	0.32231000	6.97038400
C	3.89896100	2.44170900	6.94124200
H	4.33296300	2.46302400	7.93710300
C	5.19858500	1.19141500	-5.08254700
H	5.48535500	1.51486200	-6.07905400
C	-0.30492600	-5.07990300	3.02165400
H	-1.07020300	-5.81109100	2.74630700
H	-0.61327900	-4.58185100	3.94721000
H	0.61465300	-5.63925400	3.21464500
C	0.06021000	2.94329700	-3.01595600
H	-0.99176100	3.12665200	-3.27302400
H	0.45001900	2.12458000	-3.62932200
C	3.79092500	1.41036500	-3.13660400
H	2.97840700	1.91016900	-2.61193300
C	4.16317600	1.83720000	-4.40438100
H	3.63782700	2.66606500	-4.87216500
C	1.31335800	-0.83182100	-4.60544000
H	0.35331200	-0.46576900	-4.93891900
H	2.14408800	-0.14320400	-4.55327900
Br	1.90880400	-0.62924900	-7.29236200
C	1.53134600	-2.24236400	-4.42729000
C	2.81623200	-2.73684800	-4.16281300
C	0.44290200	-3.12743800	-4.40551800
C	3.00373300	-4.07107800	-3.85133700
H	3.66187200	-2.05407800	-4.17773500
C	0.62939300	-4.45713400	-4.07374900
H	-0.55265300	-2.75507500	-4.63553500
C	1.91067800	-4.94866100	-3.77080500
H	3.99972700	-4.42755500	-3.60568000
H	-0.22441700	-5.12881600	-4.05385000
C	2.09906900	-6.34634900	-3.33882900
C	1.14382900	-6.96918300	-2.52191400
C	3.24033600	-7.07224200	-3.70865700
C	1.32609200	-8.27680900	-2.08658400
H	0.26780900	-6.41242700	-2.20044800
C	3.41709200	-8.38224700	-3.27740600
H	3.98185800	-6.61529700	-4.35822400
C	2.46251000	-8.98957100	-2.46360600
H	0.58157400	-8.73754700	-1.44311500
H	4.30215400	-8.93349100	-3.58274100
H	2.60422400	-10.01190500	-2.12463500

TS_FCaTHF_A_Brpent

Final Single point energy: -7406.225493182614

Ca	0.03918400	0.34334200	-0.52561700
F	0.53143200	-0.50376300	-2.46962200
O	-0.16228200	-1.41391900	1.03536000
O	0.02698000	2.50124500	-1.45054600
N	1.85446200	0.33042000	1.05313600
N	-2.21989400	-0.22942200	-0.15274300
C	2.97880100	1.18051700	1.01832300
C	3.04074200	-1.06120300	2.72840800
H	3.89622800	-0.39724500	2.68777500
C	-4.01845700	1.42945900	-0.32191500

C	1.94002200	-0.75147900	1.89325600
C	-3.32461500	0.31118500	-0.83413300
C	3.22262400	2.16010900	2.01365200
C	-5.17253900	1.88739900	-0.95702400
H	-5.69719500	2.74809000	-0.54582700
C	-2.49321700	-1.28954300	0.67284300
C	3.05853800	-2.18160600	3.55895400
C	-3.96287600	1.47498100	2.20029500
C	0.84146100	-2.79445500	2.74885200
C	0.86969500	-1.67700000	1.93463500
C	-3.48337900	2.13122500	0.91973700
H	-2.39319200	1.98678100	0.90190300
C	-3.78003800	-1.80649100	0.95392200
H	-4.62410100	-1.31606400	0.48379800
C	-3.71195900	3.63738900	0.85641200
C	4.35481200	2.97077300	1.92895100
H	4.54601100	3.69630000	2.71695200
C	-1.56658600	-3.04760000	2.14025400
C	-3.74127000	-0.21874800	-2.07759900
C	4.26288100	-2.51198600	4.45258900
C	4.99920700	1.93498300	-0.12189900
H	5.68115300	1.85182100	-0.96645900
C	5.25640700	2.87872600	0.87013800
C	-5.65612400	1.28910200	-2.12004100
C	3.89500900	1.08620100	-0.05704700
C	-3.97834100	-2.89207200	1.80461500
C	-3.19805300	4.33175600	-0.24699500
H	-2.68199800	3.77363800	-1.02601800
C	-5.32338000	1.35899800	2.49766100
H	-6.06128300	1.72548200	1.78769200
C	-4.90205400	0.26101300	-2.68447100
H	-5.20896400	-0.15575000	-3.64223400
C	-3.03524100	0.96575200	3.10864300
H	-1.97772300	1.00493500	2.86120800
C	-5.38169900	-3.42753600	2.12283500
C	-1.42167700	-1.94484400	1.31857900
C	-2.86546100	-3.51155200	2.39002300
H	-3.00860600	-4.37245200	3.03182300
C	-2.82616600	-1.08136100	-4.27202800
C	1.94683800	-3.03158700	3.57796500
H	1.95118900	-3.90492500	4.21900400
C	2.23935700	2.33861100	3.16500200
H	1.68941900	1.39698600	3.25627100
C	4.14379200	-1.35086500	-0.63394000
C	-4.36998000	4.36613300	1.84588900
H	-4.76404200	3.85636700	2.71987000
C	1.19953100	3.41850400	2.90137300
C	3.68541300	0.01299500	-1.11746000
H	2.60454900	-0.08344600	-1.27036800
C	-2.88313000	-1.27480500	-2.75962600
H	-1.85980400	-1.10678200	-2.39689100
C	-3.34954000	5.70723500	-0.36450200
H	-2.94731700	6.22375300	-1.23230200
C	-3.23362000	-2.69418100	-2.35573100
C	-4.52327000	5.74905800	1.73243300
H	-5.04048300	6.29599200	2.51658700
C	-0.31503900	-3.78324700	2.61548400
C	-5.74191400	0.78221900	3.69290900
H	-6.80381800	0.70311400	3.91106800
C	5.42846900	-1.54874600	-0.12225300
H	6.10865700	-0.70343600	-0.04453700
C	1.49990200	4.63310600	2.28111500
H	2.50120100	4.81023600	1.89723100
C	-3.44770800	0.38335400	4.30436400
H	-2.70812300	-0.01301500	4.99531100
C	2.93210600	2.56692100	4.50542400
C	-6.48376300	-2.66027100	1.38122200
H	-6.49621500	-1.60034800	1.66002400
H	-7.45968100	-3.08738600	1.63857200
H	-6.36118000	-2.72992900	0.29404300
C	-2.96593200	-2.13299300	-5.17784100
H	-3.16106800	-3.13697200	-4.81288200
C	4.79190900	-3.91993200	4.11586900
H	4.02807800	-4.68828400	4.27055900
H	5.65073200	-4.16240700	4.75403900
H	5.11467800	-3.96620500	3.07024900
C	-4.80451100	0.29981400	4.60530400
H	-5.13190500	-0.15243100	5.53756700
C	5.84106200	-2.81176800	0.29237600
H	6.84527800	-2.94985700	0.68467700
C	-5.64719200	-3.30353000	3.63581700
H	-4.92014100	-3.87908100	4.21799000
H	-6.64987100	-3.67891800	3.87597000
H	-5.58294300	-2.25684300	3.95099000
C	-4.01875200	6.42535600	0.62753300
H	-4.14053400	7.50137200	0.53819200
C	-0.10309400	3.21024200	3.36256900
H	-0.34259600	2.27251400	3.85890700
C	5.42188200	-1.52387400	4.26931500
H	5.78491300	-1.52251800	3.23506900
H	6.25421200	-1.81801100	4.91856100
H	5.13549700	-0.50061800	4.53494700
C	-6.93619900	1.75680400	-2.76011800
H	-7.79658900	1.19415400	-2.37554200
H	-6.91275500	1.61469800	-3.84513100
H	-7.11972200	2.81566500	-2.55279200
C	-4.53896100	-3.17958800	-2.45975600
H	-5.33210000	-2.51552900	-2.79489700
C	6.48444700	3.74810900	0.81649600
H	6.33765100	4.67594000	1.37751500
H	6.74499100	4.00360500	-0.21552200
H	7.35013100	3.23363300	1.25296900
C	0.52226600	5.61515700	2.13239500
H	0.77332100	6.55339000	1.64404100
C	3.82618400	-2.48576300	5.93019900
H	3.41416400	-1.50655300	6.19731900
H	4.68350100	-2.68818400	6.58399600
H	3.05802000	-3.23948900	6.13150100
C	-2.55852500	0.19844100	-4.77926900
H	-2.43832000	1.02852300	-4.08699900
C	4.24063500	0.42012500	-2.47418000
C	-1.08532900	4.18231200	3.20505500
H	-2.09558000	3.99235500	3.55593500
C	-0.77469400	5.39301500	2.58934400
H	-1.54396000	6.14843700	2.45430100
C	5.26905800	-0.25149400	-3.13128200
H	5.73013100	-1.11959900	-2.66911100
C	-5.48310600	-4.91109100	1.72015400

H	-5.30252300	-5.03021000	0.64688400
H	-6.48503400	-5.29501900	1.94915500
H	-4.75457600	-5.52606700	2.25803700
C	3.27204500	-2.43936000	-0.69467800
H	2.26032800	-2.29426700	-1.06905500
C	5.70200400	0.16976300	-4.39023300
H	6.50146200	-0.37121000	-4.88961500
C	-4.83275700	-4.50138300	-2.14029400
H	-5.85405100	-4.86365000	-2.22621400
C	3.27889300	3.83893000	4.97079200
H	3.02202800	4.71792100	4.38589400
C	4.96601900	-3.89438300	0.21686700
H	5.28502600	-4.87966900	0.54586100
C	0.64790900	4.20949000	-2.95824000
H	1.71845900	4.02563000	-3.10314800
H	0.28402000	4.82016800	-3.78876000
C	-2.45380900	0.42151900	-6.14596700
H	-2.24107300	1.42152700	-6.51469500
C	-2.23156000	-3.55706200	-1.91023600
H	-1.21423000	-3.18362100	-1.80861100
C	0.44127500	3.65048300	-0.64788400
H	1.45633300	3.45515900	-0.27897700
H	-0.24264200	3.73757300	0.20249200
C	3.23949100	1.46217100	5.30475600
H	2.95506600	0.47078300	4.96006600
C	-2.85978000	-1.91173300	-6.55248000
H	-2.97295400	-2.74671900	-7.23896200
C	-2.60958100	-0.63588900	-7.04314700
H	-2.52298300	-0.46436100	-8.11233400
C	-3.82305400	-5.35845800	-1.70445300
H	-4.05272100	-6.38954000	-1.44952800
C	-2.52104900	-4.88002200	-1.58474300
H	-1.72856200	-5.53545600	-1.23341600
C	3.67615600	-3.70236600	-0.27094400
H	2.98094600	-4.53621200	-0.32129200
C	0.39239600	4.84749400	-1.58809700
H	-0.59873100	5.31294500	-1.56215600
H	1.13707400	5.60144600	-1.32050400
C	3.94038300	3.99773400	6.18647000
H	4.20289000	4.99560500	6.52795000
C	0.06891300	-4.80911900	1.51859600
H	0.97619300	-5.35273100	1.80785100
H	0.25902200	-4.30242000	0.56566600
H	-0.74589200	-5.52751000	1.37071200
C	3.89851400	1.61725600	6.52118700
H	4.12754600	0.74321000	7.12567400
C	4.25726600	2.88774200	6.96581600
H	4.76889600	3.01264700	7.91616100
C	5.11022900	1.26480000	-5.00938400
H	5.43993900	1.58371600	-5.99406900
C	-0.56644900	-4.53718000	3.92655500
H	-1.36777500	-5.27069700	3.80450300
H	-0.84185300	-3.84855900	4.73255200
H	0.32315600	-5.09406000	4.23171100
C	-0.10963900	2.89600400	-2.84675300
H	-1.17783200	3.02562700	-3.06719500
H	0.29480400	2.08701500	-3.46299200
C	3.65021400	1.52029000	-3.10871200
H	2.84135700	2.04577400	-2.60355300
C	4.07573200	1.94140800	-4.36123300
H	3.59311300	2.78881900	-4.84112000
C	0.94982200	-0.71676300	-4.36316000
H	-0.00845000	-0.28854800	-4.62219700
H	1.78396400	-0.04894700	-4.20241200
C	1.14181100	-2.18992000	-4.38337800
H	0.55949400	-2.58754100	-3.53918800
H	0.66894100	-2.59968300	-5.28382000
C	2.60081800	-2.61908900	-4.26996800
H	3.06954700	-2.06979600	-3.44320200
H	3.13212400	-2.31938500	-5.18341300
C	2.77558000	-4.11502500	-4.03120900
H	2.30106500	-4.67831400	-4.84703300
H	2.24639500	-4.39491200	-3.10881400
C	4.24808200	-4.50435300	-3.91569100
H	4.72618900	-3.95594000	-3.09496100
H	4.36907100	-5.57532000	-3.72000300
H	4.78913800	-4.26571900	-4.83893400
Br	1.56884700	-0.20141200	-6.90322100

TS_FCa_THF

Final Single point energy: -4634.978707706929

Ca	4.87885600	8.92962700	13.02810900
F	5.48369800	7.82011300	11.36069100
O	4.69916300	7.87088400	15.12912700
O	4.00343700	10.98431900	10.74599500
N	6.80455300	9.27537800	14.37108600
N	2.66233900	8.25270800	13.49515900
C	7.86067100	10.14155900	14.03932100
C	8.06257300	8.50892000	16.35587800
H	8.93125200	9.06588100	16.02432100
C	0.66168700	9.51049400	12.82834100
C	6.91246200	8.56440200	15.53578100
C	1.56214200	8.43813600	12.63734900
C	8.03681000	11.37821700	14.70829700
C	-0.46424300	9.63246200	12.01231800
H	-1.14166300	10.47049100	12.16694000
C	2.43958600	7.47349600	14.59989500
C	8.11037600	7.74775300	17.52420300
C	0.34342000	10.19445500	15.24823000
C	5.80075200	7.04805600	17.13551200
C	5.79948600	7.80019000	15.97655700
C	0.95449800	10.54662000	13.90391200
H	2.04459200	10.51475500	14.05379100
C	1.21620200	6.84662400	14.92820200
H	0.38296400	7.00505400	14.25392800
C	0.62627300	11.96410700	13.44280300
C	9.07385000	12.23274300	14.33654000
H	9.21037000	13.16595100	14.88011300
C	3.40077300	6.47645200	16.64365400
C	1.36078700	7.59154400	11.52131300
C	9.36959700	7.67526100	18.40006900
C	9.75298600	10.71614400	12.61943600
H	10.42013400	10.45631400	11.79994200
C	9.94068100	11.92500500	13.28844100
C	-0.72434700	8.73294400	10.98079900
C	8.74354300	9.82319000	12.97908000
C	1.06441400	6.05371400	16.06505600
C	1.09867900	12.39054200	12.19436900

H	1.65023700	11.69295800	11.56878100
C	-1.03168800	9.99329200	15.39234600
H	-1.67764000	10.05117700	14.51970100
C	0.22245300	7.73946200	10.73081100
H	0.08286200	7.07562700	9.87928500
C	1.15443300	10.09739200	16.37952800
H	2.23024900	10.21374600	16.27305300
C	-0.26774400	5.37491100	16.41517800
C	3.51060600	7.24736600	15.50253100
C	2.16007600	5.87883400	16.91538400
H	2.06122100	5.25978900	17.80078500
C	2.52285100	6.31463300	9.67750900
C	6.97478900	7.02933600	17.90524700
H	6.99380900	6.43285800	18.81139000
C	7.05336900	11.77793400	15.80214700
H	6.67532900	10.85139200	16.24212300
C	8.99779700	7.31268600	13.13086300
C	-0.06606000	12.88167800	14.23415900
H	-0.43292600	12.58322300	15.21183700
C	5.84164400	12.51182800	15.25203400
C	8.57970200	8.48683200	12.26487000
H	7.50804600	8.34911700	12.07625700
C	2.41374400	6.54617100	11.17987000
H	3.37886300	6.97687200	11.47579500
C	0.87405400	13.68631700	11.74684900
H	1.25203300	13.99208400	10.77442900
C	2.26578000	5.26917300	11.98264900
C	-0.29307100	14.18457800	13.78726700
H	-0.83649100	14.88047100	14.42129300
C	4.58416600	6.24185000	17.57568400
C	-1.58391500	9.73013700	16.64210900
H	-2.65614300	9.57905400	16.73733100
C	10.18970400	7.31761500	13.85787200
H	10.81949900	8.20494200	13.84782100
C	5.95322000	13.56272100	14.33750200
H	6.92843000	13.81946800	13.93154100
C	0.60766900	9.83210900	17.63262900
H	1.25772100	9.75520400	18.50033600
C	7.71999100	12.53560200	16.94511900
C	-1.36095100	5.66651900	15.38005800
H	-1.56967100	6.74050300	15.30975400
H	-2.28737900	5.16127800	15.67618100
H	-1.08112300	5.30276900	14.38466400
C	2.34980400	5.07168200	9.06959200
H	2.10673300	4.20379000	9.67543300
C	9.83452800	6.21029300	18.51457700
H	9.06389200	5.57893200	18.96796700
H	10.73575100	6.14720400	19.13707500
H	10.06799900	5.80311300	17.52473000
C	-0.76670000	9.65751000	17.76932000
H	-1.19838500	9.45214800	18.74521700
C	10.57276600	6.20390300	14.60111100
H	11.50816900	6.22019300	15.15468600
C	-0.76204400	5.87711200	17.78548700
H	-0.04326000	5.64984900	18.57957400
H	-1.71445500	5.39610200	18.04166900
H	-0.91590000	6.96081100	17.76478300
C	0.17132500	14.59268000	12.54156200
H	-0.00704600	15.60629400	12.19282500
C	4.57076000	12.17285500	15.72724100
H	4.47067900	11.34819700	16.43135100
C	10.53353800	8.49607600	17.82922900
H	10.81181300	8.15232800	16.82715400
H	11.40821500	8.38607000	18.48016200
H	10.29296800	9.56335300	17.77102200
C	-1.97277300	8.84192300	10.14609900
H	-2.76651700	8.19340700	10.53877500
H	-1.78676300	8.53677100	9.11134000
H	-2.35917900	9.86579400	10.14149100
C	1.04975300	4.58655700	12.05915200
H	0.17480500	4.99556400	11.55853800
C	11.02690800	12.88117700	12.87207000
H	10.67268900	13.56635600	12.09093500
H	11.89193200	12.34671100	12.46690800
H	11.36169600	13.49321100	13.71546100
C	4.82896300	14.28359700	13.94124700
H	4.93611300	15.10083800	13.23232000
C	9.04851500	8.20565900	19.81115300
H	8.69432600	9.24181700	19.76790100
H	9.94610500	8.17627000	20.44139300
H	8.27283800	7.60452600	20.29632100
C	2.85112600	7.41001100	8.86649100
H	2.99129300	8.38467900	9.32880000
C	9.22842900	8.47281000	10.88819700
C	3.44443200	12.88463600	15.32305000
H	2.46348600	12.60832500	15.69900400
C	3.57021200	13.94969500	14.43473300
H	2.68676900	14.49540000	14.11428200
C	10.47877200	7.91153600	10.62505100
H	11.03144800	7.42490000	11.42351200
C	-0.07152300	3.84872800	16.49179900
H	0.27069100	3.45459800	15.52961300
H	-1.01883300	3.35941500	16.75091400
H	0.66836600	3.57796000	17.25209500
C	8.18140800	6.18061500	13.18708800
H	7.24231100	6.17880500	12.63627100
C	11.02711000	7.96418300	9.34336900
H	12.00264100	7.52167100	9.15905400
C	0.94869800	3.39373800	12.76834600
H	-0.00404700	2.87243600	12.81595600
C	7.79239300	13.92876700	17.01293800
H	7.32674500	14.53508500	16.24131300
C	9.75171600	5.07981600	14.65298400
H	10.04273200	4.21624900	15.24508400
C	5.84405100	11.89487200	9.52867400
H	6.77542800	11.57517900	9.05280500
H	5.47259600	12.77988100	8.99953900
C	2.99425500	7.26936900	7.49280100
H	3.25362600	8.13318100	6.88589400
C	3.37406700	4.74208100	12.64725300
H	4.32212700	5.27518400	12.60294300
C	4.56094000	12.08905300	11.49375900
H	4.44691100	11.87833700	12.56576500
H	3.99399100	13.00817400	11.28137300
C	8.30342800	11.78971500	17.97491700
H	8.23261100	10.70504100	17.93718300
C	2.48863700	4.92705200	7.68736500
H	2.34717300	3.94890400	7.23489500

C	2.80934500	6.02204000	6.89330800
H	2.92013600	5.90809400	5.81839400
C	2.06141200	2.87486300	13.42904100
H	1.98007300	1.94952700	13.99309800
C	3.27425900	3.55709300	13.37220500
H	4.14462300	3.16716000	13.89382500
C	8.54817600	5.07529500	13.94972200
H	7.89393300	4.20826600	13.99443600
C	6.00163000	12.20954800	11.02042300
H	6.42286600	13.19964500	11.21320700
H	6.64153100	11.46373000	11.51302900
C	8.44944000	14.55677700	18.07038700
H	8.49478600	15.64221700	18.10392300
C	4.94621200	4.73850100	17.55968000
H	5.78687900	4.53649600	18.23185200
H	5.22857000	4.42720100	16.54788900
H	4.09343600	4.13223700	17.88295300
C	8.95997600	12.41241500	19.03098500
H	9.40488300	11.81050300	19.81960500
C	9.03942900	13.80330500	19.08136800
H	9.54778100	14.29478500	19.90633700
C	10.33158900	8.57376100	8.30336200
H	10.75818200	8.60956200	7.30469600
C	4.19316900	6.65514800	19.01229200
H	3.33058500	6.08047500	19.36244500
H	3.93593900	7.71947800	19.04377100
H	5.01925800	6.47829100	19.70754500
C	4.78608700	10.79040700	9.53303200
H	4.11143900	10.84011800	8.67034800
H	5.23200700	9.78855500	9.58176400
C	8.53507000	9.07439300	9.83219100
H	7.55255600	9.49721100	10.02729300
C	9.07635200	9.12819500	8.55300700
H	8.51523800	9.59520000	7.74753300

TS_THF_CaBr

Final Single point energy: -7109.298795017487

Ca	0.26281800	3.51270300	4.69639600
Br	1.27325300	1.78881800	6.67727100
O	-0.34850300	5.64663900	3.83299000
O	0.29274200	3.06190300	1.48083700
N	-1.95669900	4.08903800	5.17335400
N	2.10322100	4.89926700	4.23659200
C	-2.52226300	5.17829200	4.56057600
C	-1.67675800	6.04540000	3.82599000
C	3.42550000	7.45088800	6.36986500
C	1.93639700	6.06075300	3.53594000
C	-4.52928300	1.64490800	7.49288300
C	-2.79951300	3.35326200	7.34897500
C	-2.11310000	7.18998400	3.18877900
C	3.89968600	4.99042800	5.90145400
C	3.09196000	6.00297500	6.70136800
H	2.04636000	5.85444700	6.40301800
C	-2.81908500	3.27925200	5.93665400
C	2.96274900	6.87282200	3.00937200
H	3.98438100	6.55028400	3.17518600
C	-3.65592000	2.54799300	8.09765600
H	-3.63658500	2.61925400	9.18304600
C	-3.88714700	5.53639300	4.60257600
H	-4.55148400	4.90441000	5.17983500
C	-4.37571200	6.67488400	3.95822500
C	2.68704600	8.03823500	2.29249700
C	0.61065100	6.49837400	3.29954400
C	3.15186000	5.77743800	8.20875700
C	-2.28451600	5.76644700	7.84438800
C	0.29232100	7.66206300	2.62829500
C	4.16789100	3.61953000	3.90944500
C	3.39654300	4.53876800	4.65263100
C	4.72668100	7.87865000	6.10255000
H	5.52814800	7.14715500	6.03563300
C	4.28180700	3.95219600	1.40330800
C	5.11173200	4.49865700	6.37600300
H	5.47356300	4.82692100	7.34896000
C	2.40497400	8.40468700	6.41845100
H	1.38377700	8.07929500	6.60438600
C	-3.48468400	7.48619500	3.25142200
H	-3.84980400	8.37243300	2.74291400
C	-5.86051500	7.06086900	4.01107200
C	1.35411800	8.42515700	2.11654600
H	1.12592100	9.33578800	1.57210800
C	-1.15161900	8.12345200	2.45843100
C	-4.50498600	1.53896200	6.10324900
H	-5.16140200	0.81946400	5.62038400
C	4.11957400	6.37608600	9.02115200
H	4.85682800	7.04142700	8.57986400
C	-3.66616900	2.33182000	5.32144400
C	3.18737100	5.31666200	10.98277400
H	3.19785900	5.14287000	12.05548400
C	-1.83589000	4.32764000	8.01774600
H	-0.88808900	4.23824300	7.46665800
C	2.19921400	4.95068200	8.81153000
H	1.44121300	4.47165900	8.19668900
C	3.77756500	1.64655400	2.35851900
C	-3.59664600	6.15138400	8.12712800
H	-4.31346600	5.40162300	8.45485300
C	-1.51647400	3.96332500	9.46263400
C	5.37631400	3.14390200	4.42428200
H	5.93520300	2.39809700	3.86151300
C	4.14273200	6.14211300	10.39435900
H	4.90570400	6.61580100	11.00670500
C	-1.37959200	6.73464300	7.40991300
H	-0.35760900	6.44078400	7.17639900
C	5.66310000	4.02959800	1.20381700
H	6.33755800	3.54137600	1.90181800
C	3.67290200	3.15609900	2.54715100
H	2.59921100	3.38779400	2.52497800
C	-5.47794500	0.81691300	8.31852600
H	-5.01995100	0.51493000	9.26591600
H	-5.78841900	-0.08374700	7.78044300
H	-6.38526900	1.38424300	8.56241600
C	-1.74908600	4.82361600	10.53580000
H	-2.18506400	5.80207500	10.35819000
C	2.67824400	9.75549400	6.23206000
H	1.86956200	10.48094000	6.26971300
C	5.86716200	3.57083900	5.65398900
C	-0.93764900	2.71427400	9.72484500
H	-0.73195900	2.04239300	8.89507900
C	-6.44891500	7.03528100	2.58697700

H	-7.51166900	7.30647700	2.61032000
H	-6.35987800	6.03513700	2.14697400
H	-5.93163900	7.74126600	1.92909400
C	-0.61765700	2.33163600	11.02132800
H	-0.16569900	1.35919500	11.19923400
C	-3.59641200	2.14789600	3.80926400
H	-3.30217400	3.11988000	3.39211000
C	3.74057700	10.32159100	2.28040700
H	3.87517400	10.28439300	3.36582100
H	2.78023700	10.80517300	2.07294700
H	4.53499700	10.94572500	1.85223800
C	2.21227100	4.72263500	10.18459200
H	1.45259900	4.08439000	10.62820900
C	-1.50968600	8.16103000	0.95667900
H	-2.53750200	8.51153200	0.81414800
H	-1.42091600	7.16231900	0.51501600
H	-0.83817200	8.83789900	0.41804800
C	3.79986800	8.90317600	1.68325600
C	3.98656800	10.17645800	5.99873500
H	4.20543600	11.23147100	5.85767400
C	5.00689000	9.23181500	5.92499400
H	6.02718900	9.54805700	5.72334700
C	-3.08676900	8.43582100	7.53576400
H	-3.40031100	9.46824900	7.40629500
C	6.18793700	4.71780000	0.11319500
H	7.26492900	4.76652800	-0.02509500
C	3.44151900	4.60069100	0.49572600
H	2.36706400	4.58189300	0.66356200
C	-1.42522300	4.44303300	11.83944300
H	-1.61389500	5.13025200	12.66008800
C	-0.86386900	3.19583600	12.08933400
H	-0.61177600	2.89974500	13.10402400
C	-6.00726800	8.48267000	4.58779600
H	-5.49055900	9.22495400	3.97148200
H	-5.58842500	8.53144900	5.59913500
H	-7.06687700	8.76224600	4.63792000
C	-1.77603300	8.05988400	7.24950100
H	-1.06277600	8.79925000	6.89397000
C	-3.99451800	7.47714700	7.98210200
H	-5.01997000	7.76042100	8.20504200
C	3.27700800	0.81236700	3.36618300
H	2.89059500	1.25185600	4.28429600
C	-1.29177900	9.54687800	3.04606500
H	-0.62404900	10.24616200	2.53373000
H	-1.03784100	9.54294000	4.11184400
H	-2.31610100	9.91496100	2.93511300
C	0.75712900	2.16123500	0.44394400
H	0.77573800	1.14732400	0.85455000
H	1.77968900	2.44516900	0.15770000
C	5.33826400	5.33778300	-0.80138600
H	5.74779200	5.87081900	-1.65533200
C	5.19635700	8.32826100	1.95088700
H	5.30905100	7.32597900	1.52170200
H	5.40804100	8.27061100	3.02466500
H	5.95137300	8.97739300	1.49269600
C	7.15241200	3.02397100	6.21642900
H	6.95519300	2.30924900	7.02515800
H	7.77375100	3.82237300	6.63641300
H	7.73138600	2.50510500	5.44693400
C	3.96141900	5.27819600	-0.60428400
H	3.28761900	5.76642100	-1.30352800
C	3.60686900	9.00080200	0.15783200
H	4.40283200	9.61401700	-0.28290900
H	2.64580200	9.45874100	-0.09738500
H	3.64499500	8.00745800	-0.30116800
C	-4.95154600	1.82051900	3.20917700
C	-2.49689900	1.17268000	3.39129600
C	-6.68485300	6.11103600	4.88933300
H	-7.73014300	6.43969800	4.89650000
H	-6.32484800	6.10709600	5.92453900
H	-6.66010200	5.08253200	4.51281800
C	-7.03423200	2.61684700	2.24971800
H	-7.64733600	3.44458400	1.90219200
C	3.26936100	-0.56909000	3.21632200
H	2.86858200	-1.19246300	4.01190100
C	4.27236500	1.05420300	1.19542300
H	4.65876700	1.67698700	0.39387000
C	-0.69038400	3.97302900	0.92906700
H	-0.45352000	4.98512900	1.27558500
H	-1.68637200	3.69106000	1.30484600
C	3.76948400	-1.15159500	2.05178000
H	3.76699200	-2.23169600	1.93262800
C	-1.48660600	0.77291600	4.27095500
H	-1.51056800	1.09962100	5.30827600
C	-0.59807500	3.81436100	-0.58316600
H	-1.53699700	4.06565100	-1.08453300
H	0.19639700	4.45552300	-0.98430400
C	4.27027000	-0.33315900	1.04432200
H	4.66253900	-0.77230700	0.13058200
C	-5.44077500	0.51312600	3.12835100
H	-4.81764200	-0.31539500	3.45663300
C	-5.76120300	2.86486300	2.75681400
H	-5.38222500	3.88355600	2.80844300
C	-7.51632600	1.31165100	2.18305900
H	-8.50788300	1.11299200	1.78559900
C	-6.71267900	0.26054800	2.62174500
H	-7.07731700	-0.76188900	2.56810400
C	-0.46447900	-0.08166100	3.85267500
H	0.31121000	-0.36474100	4.55839700
C	-0.21082300	2.33790000	-0.71883800
H	-1.09288800	1.70204600	-0.58044300
H	0.25026400	2.09707400	-1.68102100
C	-2.45262900	0.69445000	2.07607400
H	-3.22156900	0.99782700	1.36999400
C	-0.45034100	-0.57185100	2.55185000
H	0.33916400	-1.24457400	2.22782100
C	-1.45257400	-0.17987400	1.66624000
H	-1.44888600	-0.54916800	0.64386200

TS_THFCa_Br

Final Single point energy: -7109.294712950293

Ca	4.95864800	9.15755100	12.96210100
Br	6.00389900	7.30710600	10.28971900
O	4.81010700	7.92210500	14.94467800
O	4.85852400	10.95593500	11.47167300
N	6.91328700	9.38439700	14.25668500
N	2.75282500	8.34453800	13.30293800
C	7.99819700	10.25180000	13.99938400

C	8.10043500	8.67255400	16.30682800
H	8.96177300	9.26203200	16.01695300
C	0.65307500	9.52595500	12.78669400
C	6.99040700	8.67501500	15.43099500
C	1.59128600	8.50570600	12.50801100
C	8.09996000	11.49358300	14.67147200
C	-0.56983900	9.55382700	12.11475300
H	-1.28215000	10.34316900	12.34683000
C	2.55516500	7.51275900	14.38558200
C	8.12345400	7.92340000	17.48270300
C	0.54708500	10.19849600	15.22215800
C	5.87258100	7.11656200	16.98211200
C	5.88715500	7.87773100	15.82863700
C	0.97506200	10.59632700	13.81956100
H	2.07251800	10.66680800	13.85194200
C	1.34079300	6.85572200	14.69019400
H	0.50606400	7.01630900	14.02013800
C	0.47683900	11.98154200	13.40822700
C	9.18243500	12.33569300	14.42921200
H	9.25124500	13.27826800	14.96886200
C	3.51381100	6.46972500	16.40636700
C	1.31498600	7.62807500	11.43335100
C	9.32616000	7.93789900	18.43711400
C	10.08230800	10.77529300	12.86137000
H	10.85870200	10.48945200	12.15500800
C	10.18919900	11.99426000	13.52582100
C	-0.89251500	8.61920500	11.13433100
C	9.00943000	9.90672300	13.07399500
C	1.19268700	6.02412700	15.79769900
C	0.64085100	12.40848300	12.08411400
H	1.03981400	11.71596400	11.34956500
C	-0.79923500	10.00163200	15.54207900
H	-1.55756800	10.10673400	14.76982300
C	0.08312400	7.68886200	10.78219300
H	-0.11255500	7.00078600	9.96202900
C	1.50140300	10.04612600	16.22748800
H	2.55330700	10.16466500	15.98053800
C	-0.13623200	5.32656500	16.12159600
C	3.62257900	7.27319800	15.28608200
C	2.28442000	5.84060000	16.64917900
H	2.18828900	5.19687200	17.51678100
C	2.36028100	6.40922500	9.47654300
C	7.00824100	7.14791700	17.80531400
H	7.01280100	6.54930200	18.70996300
C	7.00863400	11.88991300	15.65462300
H	6.65690300	10.96689300	16.12657600
C	9.29774900	7.41863800	13.29126400
C	-0.05333200	12.88974900	14.32699900
H	-0.18866800	12.59154100	15.36250500
C	5.80015100	12.51075800	14.97814900
C	8.93850000	8.56307500	12.36110300
H	7.88713100	8.40540500	12.08090400
C	2.36362900	6.62085400	10.98698500
H	3.34191900	7.06840100	11.21035100
C	0.29066400	13.69510200	11.69237700
H	0.43038200	13.99885200	10.65801400
C	2.31145200	5.32614500	11.77608500
C	-0.40571400	14.18249800	13.93852900
H	-0.81408400	14.86943300	14.67520500
C	4.68530600	6.23718600	17.35234200
C	-1.18106900	9.68547300	16.84176800
H	-2.23267900	9.53860200	17.07441100
C	10.50612500	7.40873600	13.99143200
H	11.18456800	8.25467800	13.89900100
C	5.90779200	13.34568900	13.86537300
H	6.88238500	13.50616200	13.41116000
C	1.12509600	9.72675800	17.53031600
H	1.88509000	9.60946400	18.29848400
C	7.53361700	12.75994000	16.78866400
C	-1.21631400	5.60798900	15.06958600
H	-1.44670200	6.67797000	15.00541400
H	-2.13772900	5.08216400	15.34457900
H	-0.91210400	5.26034800	14.07564200
C	2.42689100	5.14822900	8.88417300
H	2.43171400	4.25915100	9.50740800
C	9.85478900	6.50391900	18.63475900
H	9.08697400	5.84674400	19.05492400
H	10.71013800	6.50811600	19.32167500
H	10.18024200	6.07909800	17.67936500
C	-0.21972400	9.55337600	17.84346800
H	-0.51800900	9.30373100	18.85814500
C	10.85116800	6.32735600	14.79637100
H	11.79865400	6.33086500	15.32934500
C	-0.65720300	5.82207300	17.48453300
H	0.05484100	5.60599500	18.28808100
H	-1.60602000	5.32770300	17.72838300
H	-0.82524900	6.90353100	17.46059500
C	-0.23570000	14.59286400	12.62041200
H	-0.51095000	15.59931800	12.31731500
C	4.53722000	12.30238400	15.54114300
H	4.44623500	11.65603000	16.41254000
C	10.48317600	8.80093200	17.91783600
H	10.85546800	8.43870200	16.95307400
H	11.31127000	8.76397700	18.63451400
H	10.19089500	9.85033200	17.79965500
C	-2.24055500	8.62553600	10.46400000
H	-2.94139800	7.96310100	10.98809100
H	-2.17192200	8.27392600	9.42976700
H	-2.67846400	9.62848400	10.46177100
C	1.14915700	4.55331100	11.82983200
H	0.25194300	4.89823800	11.32088400
C	11.34020800	12.92750800	13.25915400
H	11.08481600	13.65440500	12.47741800
H	12.22415600	12.37935200	12.91911200
H	11.60706000	13.49499100	14.15637200
C	4.78001000	13.97274500	13.33706100
H	4.88162700	14.62375900	12.47227300
C	8.88406500	8.49484900	19.80520200
H	8.48986600	9.51267800	19.70486700
H	9.73621800	8.52324600	20.49554800
H	8.10258000	7.87337300	20.25401800
C	2.37427100	7.53326100	8.63977200
H	2.32608800	8.52344600	9.08592300
C	9.70689700	8.52720700	11.04465800
C	3.41171100	12.92662400	15.01606700
H	2.43840900	12.75560500	15.46622000
C	3.52857100	13.76793000	13.91052200
H	2.64582000	14.24923000	13.49816400

C	10.64492300	7.54159300	10.73579800
H	10.88418000	6.77663400	11.46783600
C	0.07458200	3.80263200	16.19982400
H	0.43474500	3.41208200	15.24290000
H	-0.87187400	3.30457400	16.44449600
H	0.80451300	3.53748900	16.97153100
C	8.43016500	6.33560400	13.43267700
H	7.48363200	6.34161000	12.89559400
C	11.27868600	7.51877000	9.49183600
H	12.00555600	6.73981700	9.27662700
C	1.13060200	3.34622100	12.52063700
H	0.21861800	2.75531400	12.55119100
C	7.46132000	14.15393500	16.78088600
H	6.98309000	14.66507400	15.94936300
C	9.97972600	5.24712100	14.92920700
H	10.24454600	4.40545800	15.56366300
C	4.45220500	10.99787500	9.12647600
H	4.26228800	10.01681200	8.68347600
H	4.06503000	11.76284000	8.44832400
C	2.44664800	7.40273300	7.25946900
H	2.46139000	8.29169000	6.63390900
C	3.45089500	4.87129200	12.43997400
H	4.35998800	5.46814300	12.40367500
C	6.01389900	11.59813400	10.87467600
H	6.89994000	11.26205000	11.42335200
H	5.90708000	12.68407000	10.99560100
C	8.13601000	12.12758200	17.88049800
H	8.17959000	11.04075400	17.89317300
C	2.49588100	5.01189600	7.49628000
H	2.54696500	4.01824300	7.05870500
C	2.50503900	6.13531500	6.67757000
H	2.56114400	6.02889000	5.59766000
C	2.27421100	2.89966800	13.18213600
H	2.25749800	1.96093600	13.72951700
C	3.43388200	3.66896000	13.14354300
H	4.32901300	3.33304300	13.66086700
C	8.76363000	5.25827800	14.25026800
H	8.07276800	4.42558900	14.35509300
C	5.96448800	11.17718200	9.41060600
H	6.43047700	11.92593900	8.76446000
H	6.48181300	10.22305000	9.27878400
C	7.99473100	14.89746800	17.83318900
H	7.93083800	15.98224000	17.81049400
C	5.11926000	4.75551400	17.26063700
H	5.95237700	4.55583500	17.94316100
H	5.44213600	4.51894400	16.24091500
H	4.28821600	4.09253600	17.52391700
C	8.66859500	12.86515900	18.93213300
H	9.13052600	12.35220800	19.77203900
C	8.60219900	14.25803300	18.91059800
H	9.01362700	14.83911900	19.73135800
C	10.98097200	8.47866300	8.53169200
H	11.47183000	8.45909900	7.56252400
C	4.24477000	6.55097000	18.79909700
H	3.40167500	5.92157700	19.09794900
H	3.93992400	7.59972200	18.88431300
H	5.06066900	6.36952600	19.50440600
C	3.78795100	11.11888000	10.50542200
H	3.34253900	12.11119600	10.65684700
H	3.03586100	10.34949200	10.71527400
C	9.41317500	9.48502500	10.06475700
H	8.68420500	10.26020000	10.28411800
C	10.03841500	9.46515000	8.82520900
H	9.78682800	10.21854700	8.08310200

TS_THFCaF_A_Brbiphen

Final Single point energy: -7711.041002744190

Ca	-0.04048200	-0.72647700	-0.05873400
F	0.26297400	-2.17124700	1.53614300
O	-0.71327900	1.24515500	-1.22265600
O	-0.06816600	-1.95608000	-2.08485600
N	-2.20209200	-0.02232500	0.59291300
N	1.80499000	0.66695200	-0.57138700
C	-2.75076100	1.07098900	-0.02703300
C	-1.98205000	1.77485500	-0.98024600
C	2.22400200	3.35509600	1.66990700
C	1.58623900	1.81936000	-1.27917000
C	-4.85753600	-2.55422200	2.73695400
C	-3.07349400	-0.88872300	2.72302400
C	-2.42675500	2.89111000	-1.66566900
C	3.29925700	1.06835400	1.32140600
C	2.20333900	1.87416600	2.00366400
H	1.25360100	1.49390300	1.59822600
C	-3.08486800	-0.84911900	1.30909400
C	2.57631100	2.75116000	-1.67294900
H	3.59739400	2.53972700	-1.37665200
C	-3.96859400	-1.71332500	3.40449500
H	-3.95897600	-1.71444000	4.49257100
C	-4.04359400	1.59178000	0.21516900
H	-4.65657700	1.07175300	0.94168800
C	-4.51806700	2.73679800	-0.42205900
C	2.27040400	3.90406800	-2.39491800
C	0.26507800	2.13941800	-1.66480100
C	2.16533100	1.62042800	3.50829900
C	-2.52951100	1.42349100	3.60401400
C	-0.08359100	3.26930400	-2.38252400
C	4.05090800	-0.34291300	-0.50907300
C	3.05343700	0.49583500	0.04726800
C	3.40668600	4.09671700	1.67644800
H	4.35496900	3.59327500	1.84835600
C	4.10920300	-0.15911800	-3.04950200
C	4.51922300	0.85602000	1.96187800
H	4.67752400	1.28235600	2.95151500
C	1.01980800	4.01672300	1.42086700
H	0.09446000	3.44563800	1.38671200
C	-3.70455300	3.38008700	-1.36555200
H	-4.06809400	4.26468400	-1.87398200
C	-5.89320200	3.33432800	-0.09455300
C	0.93705300	4.15411400	-2.75016500
H	0.69138200	5.04052500	-3.32186400
C	-1.54660100	3.44886300	-2.78260500
C	-4.80667000	-2.57456900	1.34530800
H	-5.43073600	-3.28439800	0.80347900
C	2.45578200	2.60368300	4.45523700
H	2.72021700	3.60524300	4.12959000
C	-3.95198600	-1.73830900	0.62778500
C	2.05706900	1.04476700	6.25781800
H	2.01250100	0.81912100	7.32007000

C	-2.08529600	-0.02361600	3.49163300
H	-1.15726000	-0.01173500	2.90068100
C	1.80801800	0.34386600	3.96102900
H	1.56595400	-0.43649100	3.24014300
C	4.50077800	-2.37864700	-1.94607600
C	-3.86594400	1.77331300	3.80249100
H	-4.62521700	0.99534600	3.82585900
C	-1.72441000	-0.63035300	4.84400800
C	5.25626100	-0.53550600	0.16651000
H	6.00554900	-1.19405400	-0.26909800
C	2.40564900	2.31773900	5.82026500
H	2.63688000	3.09878900	6.53995900
C	-1.56967300	2.43647100	3.56800100
H	-0.52423400	2.16852100	3.42922400
C	5.20540300	0.70402700	-3.07939600
H	5.81396700	0.82712800	-2.18663700
C	3.79429900	-1.03024200	-1.84502500
H	2.71492300	-1.23169900	-1.88502400
C	-5.78639100	-3.46521400	3.49544200
H	-5.98954600	-3.07660000	4.49795900
H	-5.34963300	-4.46527900	3.61275300
H	-6.73994600	-3.58673100	2.97165400
C	-1.95782500	0.02208100	6.05411700
H	-2.40885500	1.01000300	6.05596400
C	0.99119200	5.39112100	1.20362800
H	0.04395600	5.88539300	1.00333300
C	5.52220400	0.07460900	1.39208100
C	-1.13249600	-1.89973700	4.87429500
H	-0.93150300	-2.41290900	3.93580400
C	-6.71593600	3.51815700	-1.38363000
H	-7.70073300	3.93804800	-1.14425500
H	-6.86375200	2.55557000	-1.88539900
H	-6.22379500	4.19682800	-2.08698700
C	-0.80326600	-2.50361500	6.08107300
H	-0.35192200	-3.49183700	6.08608200
C	-3.88211300	-1.85125700	-0.88541900
H	-2.95620300	-1.33664000	-1.17956800
C	2.97261200	6.33096600	-2.46808400
H	2.84642800	6.42062300	-1.38429500
H	2.04161800	6.64782200	-2.94765600
H	3.76306400	7.02320500	-2.78318900
C	1.75307100	0.05938600	5.31928600
H	1.45603300	-0.93208100	5.64586800
C	-1.80565100	2.59950400	-4.05299000
H	-2.85597900	2.68548200	-4.35540200
H	-1.58638500	1.54403800	-3.86272400
H	-1.16815500	2.94486500	-4.87534400
C	3.35558400	4.88943000	-2.85272200
C	2.17373300	6.12697300	1.23711600
H	2.15527500	7.20072000	1.07117700
C	3.38242500	5.47312800	1.46704100
H	4.31195600	6.03659900	1.47773200
C	-3.26891400	4.11195800	3.92021900
H	-3.55754100	5.15311200	4.03678300
C	5.52621700	1.40252600	-4.24084100
H	6.38744900	2.06554200	-4.25036200
C	3.32838200	-0.28941500	-4.20015300
H	2.47508300	-0.96386300	-4.18550600
C	-1.61651300	-0.57776000	7.26744000
H	-1.80533100	-0.04933300	8.19834000
C	-1.04315100	-1.84399800	7.28737200
H	-0.78261800	-2.31568600	8.23106700
C	-5.69096600	4.70847100	0.57418000
H	-5.16327900	5.39985700	-0.09136400
H	-5.10099400	4.60399000	1.49192800
H	-6.65993100	5.15392700	0.83269000
C	-1.93265400	3.77193600	3.71747700
H	-1.17047200	4.54609500	3.67463600
C	-4.23280900	3.10709500	3.96660500
H	-5.27768800	3.36350500	4.12168400
C	3.92153900	-3.49069000	-1.32827900
H	2.96689300	-3.37279900	-0.82374100
C	-1.87764000	4.90925300	-3.09980100
H	-1.26755900	5.26866000	-3.93311800
H	-1.70298900	5.55614000	-2.23334900
H	-2.92237400	5.00910400	-3.40658000
C	0.27340900	-3.32243700	-2.44852100
H	0.03939400	-3.96164900	-1.59276900
H	1.34894200	-3.37556100	-2.66937600
C	4.74271300	1.26406600	-5.38377300
H	4.98884900	1.81672000	-6.28636700
C	4.72189000	4.58553600	-2.22589500
H	5.09462500	3.60029900	-2.52292900
H	4.67215400	4.62147600	-1.13155800
H	5.45024300	5.33340400	-2.55963900
C	6.84278500	-0.12459600	2.08799900
H	7.24018700	-1.12862800	1.90526200
H	6.74517000	0.01747300	3.16936500
H	7.59207100	0.59251200	1.72903200
C	3.63400000	0.42024400	-5.35742900
H	3.00935800	0.31127700	-6.24018900
C	3.48884000	4.80551800	-4.38606600
H	4.27396900	5.48603700	-4.73957300
H	2.54988100	5.08200200	-4.87767100
H	3.74868700	3.78744400	-4.69510800
C	-5.00075900	-1.14865600	-1.63811700
C	-3.69901400	-3.30975800	-1.30365000
C	-6.70445400	2.44911000	0.85987900
H	-7.68079500	2.91194000	1.04343200
H	-6.20320600	2.33033200	1.82629900
H	-6.87577600	1.45336900	0.43468900
C	-5.70998200	0.06994200	-3.61768000
H	-5.45862500	0.54357900	-4.56309200
C	4.53791600	-4.73699100	-1.35253500
H	4.05842000	-5.57961800	-0.86095300
C	5.71844900	-2.55262000	-2.60805400
H	6.18534200	-1.70981900	-3.10998700
C	-0.46824500	-1.23285100	-3.29425900
H	0.22597600	-0.39869700	-3.44790500
H	-1.47075600	-0.83220100	-3.11307700
C	5.75878400	-4.89467700	-2.00660200
H	6.24523900	-5.86591600	-2.03138100
C	-2.68756000	-4.05571900	-0.68272800
H	-2.08521900	-3.59075600	0.09623200
C	-0.45009200	-2.25885200	-4.42740400
H	-1.26894800	-2.09255600	-5.13220900
H	0.49611200	-2.20786800	-4.97694000
C	6.34359700	-3.79869200	-2.63482800

H	7.29196000	-3.91065000	-3.15388200
C	-6.31986600	-1.12326100	-1.18232200
H	-6.56922800	-1.56836400	-0.22406800
C	-4.71274200	-0.54092800	-2.86410100
H	-3.68835400	-0.54011800	-3.22977400
C	-7.02522800	0.07780900	-3.15782100
H	-7.80758100	0.55583600	-3.74107500
C	-7.32362400	-0.51805300	-1.93549800
H	-8.34324300	-0.50571300	-1.55902900
C	-2.45225300	-5.37844800	-1.03415000
H	-1.65921000	-5.93507300	-0.54035700
C	-0.55835900	-3.59666100	-3.68599400
H	-1.59577900	-3.80516500	-3.40105200
H	-0.17150600	-4.43877400	-4.26619900
C	-4.46892900	-3.92826200	-2.28849000
H	-5.25907800	-3.37188800	-2.78463400
C	-3.22947700	-5.98857800	-2.01970600
H	-3.04998500	-7.02403100	-2.29568500
C	-4.23620600	-5.25888600	-2.64273700
H	-4.85011300	-5.72348000	-3.41002400
C	1.15584300	-3.94049700	1.62587600
H	1.42338300	-3.81193800	0.59076400
H	0.20794200	-4.40224300	1.85590900
Br	1.82736200	-6.50637800	1.06607500
C	2.09331500	-3.63927300	2.67310000
C	3.27697000	-2.93678500	2.39764800
C	1.79461000	-3.96717000	4.00422900
C	4.12313000	-2.56290700	3.42466800
H	3.51639200	-2.65159100	1.37643900
C	2.64603500	-3.59721500	5.02894300
H	0.89021800	-4.52956000	4.22047200
C	3.82166300	-2.87636800	4.75993200
H	5.00730900	-1.97856500	3.19291600
H	2.40521900	-3.87620200	6.05058400
C	4.70790000	-2.43247300	5.85159000
C	4.18073900	-2.07107700	7.10046300
C	6.09503100	-2.34331000	5.66075700
C	5.01389000	-1.63186800	8.12275900
H	3.10723900	-2.10481500	7.26277100
C	6.92655400	-1.90791500	6.68602400
H	6.52835000	-2.64014500	4.70960800
C	6.39005300	-1.54836300	7.92092600
H	4.58495800	-1.34429900	9.07871500
H	7.99923500	-1.85492100	6.52169600
H	7.04026500	-1.20513800	8.72061700

TS_THFCaF_A_Brpent

Final Single point energy: -7406.231138483161

Ca	-0.02398200	-0.70051300	-0.15364100
F	0.63513700	-2.02347700	1.43529800
O	-0.68701600	1.32819500	-1.26485800
O	-0.30842900	-2.22487200	-1.92625300
N	-2.14968700	0.02920100	0.55327600
N	1.82670900	0.65288300	-0.70344300
C	-2.66201600	1.19279100	0.04053600
C	-1.91073500	1.90703200	-0.91607000
C	2.83540000	3.30550900	1.57659200
C	1.62888000	1.82630100	-1.37933800
C	-4.85168400	-2.45046400	2.68836200
C	-2.96994200	-0.89815800	2.67347100
C	-2.33221700	3.07961800	-1.51673000
C	3.57697400	0.93248200	0.98719200
C	2.64376800	1.81470900	1.80028900
H	1.63160200	1.58941800	1.43688100
C	-3.03884100	-0.79098900	1.26537900
C	2.64338300	2.70976700	-1.81812300
H	3.66853400	2.43285100	-1.59988100
C	-3.88391400	-1.69978000	3.35607500
H	-3.82416700	-1.76062200	4.44107600
C	-3.89777400	1.77832800	0.40300900
H	-4.48964900	1.25662200	1.14628400
C	-4.33971900	2.98464400	-0.13737400
C	2.35848100	3.88842600	-2.50359300
C	0.30850500	2.21163000	-1.69408600
C	2.65913600	1.44123300	3.27957100
C	-2.23389900	1.32118800	3.64672300
C	-0.02156900	3.38212600	-2.35347900
C	3.98116000	-0.49511700	-0.93661000
C	3.12565400	0.38898100	-0.23963100
C	4.09656100	3.89524900	1.47482500
H	4.98522900	3.27001900	1.48082600
C	3.81344500	-0.27756400	-3.43879800
C	4.85629800	0.63231000	1.45430200
H	5.17476500	1.03370400	2.41549800
C	1.70808000	4.13059500	1.53855900
H	0.71858700	3.68143800	1.59202900
C	-3.55323700	3.62801000	-1.10460400
H	-3.89161700	4.55967200	-1.54106000
C	-5.64327200	3.64890100	0.32709800
C	1.02042000	4.22740300	-2.75445500
H	0.78848900	5.14567700	-3.28073200
C	-1.49419300	3.63063400	-2.66936200
C	-4.84861000	-2.42122900	1.29496400
H	-5.53011300	-3.07322600	0.75009200
C	3.14743600	2.28429000	4.27803800
H	3.54815500	3.25895700	4.01456900
C	-3.96689600	-1.61199500	0.57903500
C	2.58908300	0.65765800	5.97739400
H	2.55176700	0.35765700	7.02126600
C	-1.88473700	-0.13813300	3.42183900
H	-1.00574400	-0.13593200	2.76062600
C	2.13385800	0.19669800	3.65195300
H	1.74202300	-0.47204300	2.88657700
C	3.89079200	-2.59391600	-2.39448700
C	-3.50686800	1.71431300	4.06330600
H	-4.28498600	0.96462900	4.18644300
C	-1.44802700	-0.84991400	4.69725900
C	5.26176200	-0.75416600	-0.44905600
H	5.90698000	-1.44255300	-0.99240100
C	3.11847600	1.89235000	5.61754300
H	3.50456200	2.56349700	6.38045700
C	-1.25073000	2.29814400	3.47950300
H	-0.25411200	1.99812800	3.15962700
C	5.13518800	0.01821600	-3.78267800
H	5.94805500	-0.35303400	-3.16368200
C	3.48637300	-1.13367100	-2.22554000
H	2.38807200	-1.13063300	-2.15279800
C	-5.85247400	-3.27953100	3.44830200

H	-6.74774600	-2.69238600	3.69032700
H	-5.43415300	-3.64000400	4.39332500
H	-6.17835600	-4.14375600	2.86103400
C	-1.43238000	-0.23415500	5.94803900
H	-1.76222900	0.79584800	6.04740900
C	1.83377300	5.51134900	1.42208400
H	0.94293800	6.13316400	1.38659000
C	5.72813900	-0.18516600	0.73582800
C	-1.00686600	-2.17646400	4.60342500
H	-1.01638400	-2.66643900	3.63247800
C	-6.53007900	3.99938200	-0.88273600
H	-7.46132300	4.46754100	-0.54084300
H	-6.78388300	3.09657300	-1.44864400
H	-6.03396000	4.69900900	-1.56217800
C	-0.56464300	-2.86601600	5.72497600
H	-0.22239500	-3.89317600	5.62645700
C	-3.93354100	-1.66472100	-0.93909800
H	-2.94914300	-1.26241500	-1.21967300
C	3.29893300	6.22173500	-2.41979500
H	3.36198800	6.18024000	-1.32765600
H	2.33218200	6.65924700	-2.68891000
H	4.08787900	6.88896000	-2.78890400
C	2.09235400	-0.18893200	4.98597100
H	1.65054600	-1.14414700	5.25691100
C	-1.85076400	2.81646900	-3.93972700
H	-2.91354900	2.93821700	-4.17978200
H	-1.65073300	1.75057800	-3.78626300
H	-1.25216500	3.16386400	-4.79002600
C	3.46784500	4.81447500	-3.02171500
C	3.09816700	6.09200900	1.34613900
H	3.20157900	7.16993800	1.25547300
C	4.22776900	5.27760400	1.36457000
H	5.21791700	5.71940500	1.28721700
C	-2.80214400	4.02334300	4.14135800
H	-3.02487300	5.07043200	4.32795700
C	5.42229900	0.77816800	-4.91229500
H	6.45600500	0.99888900	-5.16552800
C	2.78702600	0.21526400	-4.24469000
H	1.75370100	0.01455500	-3.97163300
C	-0.98872900	-0.92417600	7.07756900
H	-0.98267400	-0.42350700	8.04232500
C	-0.55344200	-2.24044500	6.97279300
H	-0.20675200	-2.77693200	7.85181300
C	-5.29597000	4.94648800	1.08349900
H	-4.75893300	5.64865400	0.43672000
H	-4.66082700	4.72924600	1.94976800
H	-6.21054900	5.43813100	1.43859700
C	-1.53028000	3.64093600	3.72000700
H	-0.75373400	4.38873500	3.57939100
C	-3.78870900	3.05469600	4.31356800
H	-4.78560400	3.34560500	4.63471200
C	3.90945600	-3.44590300	-1.28313300
H	3.72146100	-3.03336600	-0.29597500
C	-1.78594800	5.10722400	-2.94266000
H	-1.19910000	5.46220000	-3.79441200
H	-1.55409800	5.73128100	-2.07285100
H	-2.83914100	5.24700900	-3.20249100
C	0.26508900	-3.57289900	-1.99205500
H	-0.22706200	-4.19385300	-1.23778400
H	1.33453700	-3.49271200	-1.76594500
C	4.38919000	1.25661300	-5.71725000
H	4.61337400	1.85250800	-6.59782700
C	4.86949400	4.30519400	-2.66437700
H	5.06339000	3.31907100	-3.10251200
H	5.00808500	4.23505400	-1.57929800
H	5.61954700	5.00154700	-3.05603100
C	7.12783900	-0.45291100	1.22119200
H	7.40443100	-1.50309600	1.07996600
H	7.23272600	-0.20929100	2.28251800
H	7.85719800	0.15245500	0.66807700
C	3.06890200	0.97484500	-5.37787500
H	2.25466700	1.35518600	-5.98932200
C	3.37225200	4.91340100	-4.55696900
H	4.17611300	5.55095600	-4.94592400
H	2.41566300	5.34377400	-4.87031600
H	3.46641800	3.92181500	-5.01313300
C	-4.95236800	-0.77309400	-1.62721300
C	-3.95772300	-3.10214600	-1.45359500
C	-6.45995700	2.74739100	1.26167300
H	-7.38810600	3.25926300	1.54011300
H	-5.91607200	2.51685600	2.18407100
H	-6.72604300	1.80304600	0.77230700
C	-5.49035200	0.72407500	-3.46066000
H	-5.17188500	1.27862700	-4.33948700
C	4.16016900	-4.80631700	-1.42314600
H	4.15859700	-5.44503600	-0.54398800
C	4.12668600	-3.15009300	-3.65445000
H	4.10987400	-2.51436800	-4.53513600
C	-0.78086300	-1.83907400	-3.24949800
H	-0.58780200	-0.76787500	-3.37423900
H	-1.86267300	-2.02566900	-3.30449500
C	4.39683800	-5.34898600	-2.68534600
H	4.59178600	-6.41192500	-2.79764000
C	-3.05666500	-4.02426900	-0.90469500
H	-2.40044500	-3.70840800	-0.09610000
C	-0.01903700	-2.73766600	-4.20667900
H	-0.52506500	-2.83335200	-5.17106200
H	0.99365600	-2.35090100	-4.37319900
C	4.37818500	-4.51435100	-3.79861300
H	4.55825500	-4.92358600	-4.78937100
C	-6.27598500	-0.68151100	-1.19357000
H	-6.58858100	-1.21548600	-0.30057600
C	-4.57261600	-0.05894800	-2.76655200
H	-3.53992900	-0.10834400	-3.10587700
C	-6.81141000	0.80079800	-3.02506100
H	-7.53054900	1.41347500	-3.56199500
C	-7.19888500	0.09812200	-1.88657000
H	-8.22413200	0.16192700	-1.53109300
C	-2.99347700	-5.33110000	-1.37080200
H	-2.28122100	-6.02573200	-0.93209900
C	0.02704000	-4.05103600	-3.41878200
H	-0.93571300	-4.57022400	-3.49059400
H	0.81941100	-4.72640400	-3.75290100
C	-4.79642100	-3.52974600	-2.48361600
H	-5.50207300	-2.83402800	-2.92835200
C	-3.83872900	-5.74913700	-2.39983600
H	-3.79296800	-6.77134500	-2.76526900
C	-4.73892400	-4.84413400	-2.95117400

H	-5.40434700	-5.15685000	-3.75169700
C	1.07412200	-3.94501100	1.60902400
H	1.54769800	-3.85757500	0.64431500
H	0.01588300	-4.15915300	1.64185500
C	1.86393300	-3.82784200	2.86249400
H	1.34385600	-3.10307400	3.50324200
H	1.81878400	-4.78180300	3.40098500
C	3.30918200	-3.39398400	2.64631100
H	3.31523900	-2.40807400	2.15950000
H	3.80413000	-4.09495000	1.95861000
C	4.09579700	-3.31965500	3.95354300
H	4.18153500	-4.32780700	4.38201300
H	3.53063300	-2.71878900	4.67924100
C	5.48031600	-2.70815600	3.76022100
H	5.39395500	-1.68029800	3.38860400
H	6.04597400	-2.68429500	4.69773400
H	6.06381600	-3.27737700	3.02654300
Br	1.32301100	-6.48655600	1.07101000

TS_THF_CaF

Final Single point energy: -4634.984396056421

Ca	0.37931500	3.43919700	4.55496800
F	1.03956300	2.32601700	6.19890700
O	-0.31995500	5.64549700	3.83310500
O	0.46046300	3.64909900	1.00623900
N	-1.82568500	4.03230200	5.22630100
N	2.18044000	4.88003400	3.97273700
C	-2.42885800	5.14639000	4.71878400
C	-1.64210900	6.04563200	3.95367600
C	3.22310600	7.69567900	5.98951800
C	1.92620100	6.05179700	3.31239300
C	-4.18471300	1.39508200	7.55662000
C	-2.48565200	3.13361600	7.39927100
C	-2.12740500	7.21909500	3.41131200
C	3.95066900	5.28212300	5.61170300
C	3.02859100	6.23326800	6.35880500
H	2.00936700	5.97182200	6.04341800
C	-2.62377200	3.17057200	5.99503700
C	2.89585000	6.87258900	2.69909300
H	3.93007100	6.55647400	2.77514800
C	-3.26564100	2.25630800	8.15289300
H	-3.14859900	2.24105100	9.23475300
C	-3.78305700	5.50932900	4.89817100
H	-4.39692600	4.85077900	5.50142100
C	-4.31582400	6.68207800	4.36123300
C	2.55605200	8.04167300	2.01548800
C	0.58373800	6.49458000	3.21462900
C	3.08317100	6.01660400	7.86715200
C	-2.00336300	5.49961800	8.09502400
C	0.20932200	7.67451000	2.60168800
C	4.37110900	3.79085100	3.74120200
C	3.49744900	4.67155900	4.41050800
C	4.47904000	8.24611100	5.72991000
H	5.35496200	7.60292300	5.71836900
C	4.83341700	3.46571500	1.29828500
C	5.21616100	4.98953500	6.10797600
H	5.52873200	5.43654900	7.05100400
C	2.10945000	8.53949000	5.97626000
H	1.12300400	8.11561000	6.15131000
C	-3.48459300	7.52285400	3.61611800
H	-3.88352500	8.43762000	3.18997900
C	-5.78818600	7.06551800	4.56390200
C	1.21507700	8.43412700	1.97995600
H	0.93263500	9.34824500	1.46842800
C	-1.22901400	8.18213300	2.64129600
C	-4.28341400	1.40241000	6.16440900
H	-4.97400200	0.71490000	5.68177100
C	3.71469100	6.90578300	8.73864300
H	4.18170500	7.80454300	8.34557600
C	-3.51653100	2.26268300	5.38173900
C	3.14126500	5.51918800	10.63186100
H	3.15711100	5.32781900	11.70158600
C	-1.48438400	4.07411100	8.05712600
H	-0.60560600	4.08603100	7.39768900
C	2.47668600	4.87261900	8.40097500
H	1.97804100	4.16778900	7.73512700
C	3.72115600	1.59783300	2.63240700
C	-3.29907100	5.79175900	8.52691500
H	-3.95643400	4.98063000	8.83227600
C	-0.99527900	3.55404300	9.40029000
C	5.64316300	3.53647300	4.26179900
H	6.30190600	2.84660600	3.73827400
C	3.74831100	6.65723800	10.11083500
H	4.24588500	7.36215600	10.77199400
C	-1.17962700	6.55097800	7.69015900
H	-0.17133100	6.33028700	7.34349200
C	6.01825000	2.77182800	1.02982400
H	6.28254800	1.90317100	1.62713300
C	3.92104100	3.10001400	2.46002400
H	2.93261100	3.52418700	2.22909000
C	-5.05495100	0.49176800	8.39003000
H	-4.54120500	0.17920500	9.30463200
H	-5.34582300	-0.40379700	7.83224500
H	-5.97799600	1.00297500	8.69264400
C	-1.20971300	4.21643000	10.60782400
H	-1.74604900	5.16102300	10.61803400
C	2.24353200	9.90035400	5.72106100
H	1.36223900	10.53653300	5.70470200
C	6.08830600	4.12489700	5.44039600
C	-0.28279300	2.34712900	9.41677200
H	-0.08481900	1.84211700	8.47365700
C	-6.49985100	7.08957000	3.19760900
H	-7.55616300	7.35994700	3.32012800
H	-6.45007200	6.10314600	2.72113800
H	-6.03737200	7.81577500	2.52126400
C	0.18286900	1.80952700	10.60965600
H	0.73701900	0.87431700	10.59995100
C	-3.55427200	2.20568200	3.86159800
H	-3.46650100	3.24169700	3.50720400
C	3.49176400	10.35714900	1.61542800
H	3.64260100	10.50518900	2.69007900
H	2.51363500	10.76811300	1.34763900
H	4.25475500	10.93135300	1.07573300
C	2.50260800	4.62800800	9.76967300
H	2.01012400	3.74457600	10.16582400
C	-1.76815400	8.36118000	1.20499800
H	-2.78829800	8.75811200	1.22307700
H	-1.78100100	7.40283000	0.67517300

H	-1.14209800	9.05947800	0.64026100
C	3.60545000	8.86445500	1.25616600
C	3.50435500	10.44339700	5.47963400
H	3.61411600	11.50587800	5.27974300
C	4.61981000	9.60970100	5.48003700
H	5.60584500	10.02093900	5.27913000
C	-2.93362100	8.14693900	8.14017000
H	-3.29685100	9.17105500	8.14863300
C	6.85444400	3.16420600	-0.01136200
H	7.77055900	2.61151800	-0.20237100
C	4.50353000	4.55433500	0.48688100
H	3.58531900	5.10339200	0.68571900
C	-0.73615300	3.68167500	11.80776500
H	-0.91121000	4.21542700	12.73830500
C	-0.04452600	2.47540200	11.81571700
H	0.32332600	2.05914700	12.74967400
C	-5.87792400	8.46263700	5.20750700
H	-5.42225200	9.23071200	4.57490600
H	-5.36287900	8.47008100	6.17498100
H	-6.92724000	8.73730600	5.37160900
C	-1.64038000	7.86511900	7.70474600
H	-0.99134500	8.67149800	7.37242700
C	-3.75965300	7.10527200	8.55783500
H	-4.77170300	7.31506200	8.89454600
C	3.55231700	1.02770700	3.89717600
H	3.60116600	1.65688300	4.78128300
C	-1.24367200	9.55369100	3.35692700
H	-0.61553900	10.27565400	2.82540900
H	-0.86159800	9.44970900	4.37863500
H	-2.26026200	9.95627700	3.40644100
C	0.99587100	2.98112900	-0.15947600
H	1.12287400	1.91768900	0.07432400
H	1.98209100	3.41248700	-0.38733400
C	6.51767600	4.25532000	-0.81059800
H	7.16799600	4.55831500	-1.62660000
C	5.03808500	8.41143300	1.56576300
H	5.21411800	7.37769300	1.24906200
H	5.25821100	8.48720600	2.63699900
H	5.74629600	9.05039100	1.02606000
C	7.46429700	3.84978600	5.98647900
H	7.42794400	3.62867300	7.05898500
H	8.12145500	4.71922700	5.85896200
H	7.93087600	3.00186700	5.47642700
C	5.33576400	4.94697400	-0.55919400
H	5.05844200	5.79435200	-1.18090900
C	3.35830000	8.69192600	-0.25596600
H	4.10924900	9.24476300	-0.83456500
H	2.36649800	9.06204500	-0.53704400
H	3.41747400	7.63373900	-0.53579200
C	-4.87494400	1.68372200	3.32811800
C	-2.35513900	1.46506200	3.27489700
C	-6.53243100	6.08198100	5.47622100
H	-7.57095500	6.41117100	5.59418700
H	-6.07713800	6.03649900	6.47216600
H	-6.54744600	5.06903900	5.05899600
C	-7.14666000	2.14377600	2.61164000
H	-7.93399200	2.86335600	2.40253200
C	3.33156100	-0.34131400	4.04196700
H	3.20410600	-0.75944600	5.03731700
C	3.63837700	0.75970500	1.51282400
H	3.75466900	1.18222200	0.51838200
C	-0.68632000	4.43913000	0.62538900
H	-0.63456900	5.39148600	1.16206800
H	-1.60671200	3.91235100	0.92354500
C	3.27529600	-1.16705400	2.92386600
H	3.11131400	-2.23538500	3.03630300
C	-1.32814400	0.94211400	4.06583600
H	-1.38533700	1.02373000	5.14884100
C	-0.59639200	4.58914500	-0.88724000
H	-1.56856300	4.78821300	-1.34757000
H	0.08898100	5.40570400	-1.14580700
C	3.42611800	-0.60727200	1.65576500
H	3.37436500	-1.23825400	0.77199200
C	-5.11163200	0.32044400	3.13262700
H	-4.31629700	-0.39481600	3.32919800
C	-5.90466800	2.58764700	3.05788500
H	-5.72329700	3.65159200	3.19733400
C	-7.37558900	0.78181400	2.42676600
H	-8.34236800	0.43159200	2.07575800
C	-6.35254900	-0.12790100	2.68755600
H	-6.52079600	-1.19182000	2.54296100
C	-0.23559600	0.29413100	3.48346500
H	0.55201800	-0.10523900	4.11640500
C	0.00326400	3.23819400	-1.29145000
H	-0.77649300	2.46776600	-1.29953800
H	0.48824400	3.25306000	-2.27181900
C	-2.26655700	1.31144700	1.88615800
H	-3.06066500	1.70660500	1.25636700
C	-0.16466000	0.14277200	2.10181500
H	0.68325000	-0.36556700	1.65303700
C	-1.18952300	0.65224700	1.30644800
H	-1.14550400	0.53924500	0.22663100

TS_THF_CaTHF

Final Single point energy: -4767.379707016064

Ca	4.82916400	9.05582500	13.05319900
O	4.70928900	7.79282300	15.02759300
O	5.02391500	10.64793400	11.35955300
N	6.78263000	9.27761500	14.33246500
N	2.64945100	8.29090700	13.46945000
C	7.83156000	10.20361500	14.13394400
C	8.11783900	8.30188300	16.17261000
H	8.98501200	8.86196000	15.84326900
C	0.72256200	9.56596800	12.62059300
C	6.93314600	8.44609700	15.41947500
C	1.55841000	8.42658200	12.58356200
C	7.92662400	11.36631600	14.94219800
C	-0.34296100	9.68225500	11.72723600
H	-0.95477000	10.58251900	11.74865000
C	2.41123100	7.54741400	14.60259900
C	8.20020200	7.45126100	17.27498200
C	0.16346600	10.43768000	14.91980400
C	5.85219100	6.84960200	16.95790700
C	5.83163600	7.66213900	15.84014500
C	0.97329300	10.65685300	13.65079100
H	2.02746000	10.55739100	13.94706300
C	1.15401200	7.05052300	15.00578200
H	0.30336900	7.28553600	14.37700200

C	0.82100400	12.05566800	13.06237000
C	8.97177700	12.26479000	14.75389300
H	9.04697800	13.13263500	15.40744900
C	3.39288400	6.47222600	16.59332100
C	1.30343700	7.44222600	11.59669200
C	9.50476200	7.26617100	18.06114900
C	9.82071900	10.95488400	12.95045100
H	10.55004600	10.79987300	12.15780000
C	9.92875600	12.08439700	13.75293300
C	-0.63367900	8.68848900	10.79561400
C	8.80554800	10.01041600	13.13311900
C	0.99206100	6.29364500	16.16536900
C	1.51211100	12.36239400	11.88314200
H	2.09515300	11.58225400	11.39694900
C	-1.23275400	10.37559000	14.89622900
H	-1.76057400	10.45143300	13.94941300
C	0.21273800	7.58237000	10.73933600
H	0.03908700	6.82650700	9.97553400
C	0.81342400	10.31600500	16.14891500
H	1.90042000	10.31821600	16.17960400
C	-0.38222900	5.78557300	16.62289600
C	3.49911400	7.24828000	15.45539500
C	2.11858400	5.99720000	16.93855800
H	2.01375900	5.38213000	17.82582600
C	2.52821000	5.88768900	10.00280600
C	7.05939200	6.74616300	17.66611200
H	7.10081100	6.09468900	18.53276600
C	6.86022700	11.65439100	15.99195900
H	6.42764400	10.69299400	16.28647900
C	9.68976200	7.67924100	12.93701900
C	0.07917000	13.06665400	13.67382100
H	-0.45564000	12.86242400	14.59652500
C	5.72082700	12.47991300	15.41737200
C	8.80057900	8.73792200	12.30015100
H	7.77792500	8.33572400	12.34624200
C	2.23937600	6.25091300	11.45913900
H	3.19638600	6.57900100	11.88866300
C	1.45766500	13.63554100	11.32962500
H	2.00281100	13.85326400	10.41467600
C	1.80771200	5.04341700	12.27573900
C	0.01753500	14.34518400	13.11742700
H	-0.56918200	15.11551600	13.61102900
C	4.61469900	6.08834200	17.42197600
C	-1.95894400	10.22552200	16.07376200
H	-3.04427300	10.18309300	16.03527800
C	11.07675600	7.84121300	13.01501200
H	11.54069500	8.73539000	12.60697200
C	5.94472400	13.63734800	14.66573500
H	6.96196600	13.93363100	14.42426100
C	0.09157600	10.16588700	17.33050000
H	0.61892300	10.06868200	18.27584700
C	7.45547700	12.26027600	17.26015800
C	-1.50714800	6.21319000	15.67267600
H	-1.58411500	7.30453600	15.60617500
H	-2.46353100	5.82952600	16.04534700
H	-1.35489800	5.81489800	14.66272700
C	2.65416000	4.56323900	9.57447700
H	2.49136500	3.75157100	10.27722000
C	9.91699600	5.78157100	18.02620700
H	9.15153500	5.14122700	18.47585800
H	10.85155600	5.63581900	18.58162200
H	10.07490300	5.45159900	16.99337600
C	-1.29950400	10.12780500	17.29755900
H	-1.86654600	10.00954700	18.21689900
C	11.87487100	6.86455600	13.60186200
H	12.95099300	7.00773700	13.65321200
C	-0.69549500	6.35049400	18.02195000
H	0.04392800	6.02445400	18.76057200
H	-1.68300300	6.00861600	18.35614400
H	-0.69853700	7.44544600	18.00197200
C	0.70338000	14.63581300	11.94356100
H	0.65601400	15.63107700	11.51039000
C	4.40168400	12.11028800	15.69401800
H	4.21477500	11.21463400	16.28486500
C	10.66144900	8.09114900	17.48224300
H	10.87651300	7.80959100	16.44496100
H	11.56607500	7.91208800	18.07391100
H	10.45094200	9.16640100	17.51108900
C	-1.81959900	8.80577000	9.87590200
H	-2.70857600	8.34218900	10.32216900
H	-1.63323600	8.30244700	8.92218300
H	-2.06379600	9.85340000	9.67501900
C	0.54859000	4.46373700	12.10316300
H	-0.16476100	4.92084200	11.42212600
C	11.02266800	13.09630000	13.54141600
H	10.64585100	13.97787800	13.00756200
H	11.84210900	12.67678700	12.95059600
H	11.42761000	13.44614600	14.49674600
C	4.87974800	14.41531600	14.22019500
H	5.07509900	15.31293500	13.63898800
C	9.29099300	7.69213800	19.52626900
H	8.97861900	8.74081000	19.58411900
H	10.22343000	7.57868100	20.09248500
H	8.52233700	7.08315200	20.01279100
C	2.75136000	6.90480900	9.06722900
H	2.66046500	7.94163700	9.37997800
C	9.08740900	8.97517300	10.82326900
C	3.33444300	12.88847300	15.25014600
H	2.31506700	12.59444500	15.48068000
C	3.56888400	14.04439500	14.51165400
H	2.73305100	14.64040400	14.15580300
C	9.74303600	8.02304100	10.03848500
H	10.14324100	7.12642300	10.50301700
C	-0.37513800	4.24742300	16.69660900
H	-0.15933500	3.81844600	15.71296900
H	-1.35435900	3.88046400	17.02832000
H	0.37968700	3.88085400	17.40005100
C	9.12490600	6.52070100	13.46936200
H	8.04599000	6.39506200	13.44242500
C	9.87918800	8.20159000	8.66278000
H	10.39083600	7.44571000	8.07273700
C	0.20330700	3.29893200	12.78185900
H	-0.77981000	2.85967800	12.63388800
C	7.29112400	13.59428800	17.63372800
H	6.68909100	14.25990600	17.02250100
C	11.29941300	5.70513300	14.12113100
H	11.92331800	4.94267300	14.57962400
C	4.64886800	12.04105000	9.48504900

H	4.95106300	12.20403100	8.44709100
H	3.59688800	12.32416900	9.59006500
C	3.08056000	6.61176600	7.74906900
H	3.24818800	7.42200100	7.04385700
C	2.70329700	4.44370400	13.16227900
H	3.67510900	4.90119400	13.33141700
C	5.32743400	12.02152300	11.77540100
H	6.21931800	11.99385300	12.41104100
H	4.47397900	12.39187100	12.35640700
C	8.22116900	11.42693800	18.08493000
H	8.33980200	10.38138700	17.80753900
C	2.98368400	4.26509900	8.25230600
H	3.07227400	3.22651900	7.94449200
C	3.19655300	5.28613700	7.33219800
H	3.44976600	5.05447200	6.30128200
C	1.11430500	2.69479200	13.64681200
H	0.84523900	1.78410700	14.17507600
C	2.36333300	3.27718000	13.84339000
H	3.07435400	2.82612500	14.53084700
C	9.92014500	5.53626300	14.05237000
H	9.45703900	4.64171800	14.46047000
C	5.52243600	12.80664300	10.48539400
H	5.22098000	13.85106400	10.60220500
H	6.57219100	12.77983800	10.17310400
C	7.89173700	14.08819000	18.79308900
H	7.75204900	15.13109600	19.06532800
C	4.86193400	4.57077200	17.26379700
H	5.73317900	4.25912000	17.84993600
H	5.04275300	4.32167500	16.21219700
H	3.99049300	4.00383100	17.60837700
C	8.82111200	11.91629800	19.23867400
H	9.41271500	11.25153600	19.86308000
C	8.66177400	13.25533400	19.59733400
H	9.12866800	13.64089600	20.49946900
C	9.36089400	9.33581900	8.04467000
H	9.46711700	9.47440500	6.97236300
C	4.35271300	6.40851300	18.90992400
H	3.48358700	5.85786700	19.28040400
H	4.16718800	7.47977200	19.04181900
H	5.21073600	6.12793400	19.52736500
C	4.85683800	10.59791500	9.90998500
H	4.00785400	9.94233200	9.69499900
H	5.77089700	10.17783800	9.47377800
C	8.57476400	10.11430000	10.19042500
H	8.06091400	10.86442300	10.78532400
C	8.70739500	10.29439600	8.81804000
H	8.29703600	11.18579500	8.34994600
O	5.67267700	7.10787200	11.04021700
C	6.16845600	7.28219800	9.67882900
C	5.88532400	5.73535900	11.44642400
C	6.71082900	5.92084000	9.24758200
H	5.34276300	7.62651900	9.04876800
H	6.95522800	8.04273100	9.70535000
C	7.03713200	5.24863600	10.58566600
H	6.08516200	5.73148300	12.52388200
H	4.97610400	5.14764000	11.24764000
H	7.58360300	6.02471900	8.59692800
H	5.93959200	5.35140200	8.71589400
H	7.99018100	5.61785700	10.98314400
H	7.07707400	4.15764300	10.52102000

TS_THFCa_THF

Final Single point energy: -4767.377890184465

Ca	4.85683800	8.92464000	13.03405300
O	4.75593300	7.63387200	14.97026600
O	5.02594100	10.83908900	10.83704400
N	6.79696700	9.20669000	14.33089400
N	2.65293600	8.27679100	13.51338500
C	7.83673300	10.14920600	14.14929000
C	8.11940800	8.26475500	16.19667700
H	8.96757100	8.87203800	15.90484000
C	0.77085200	9.60245300	12.64134800
C	6.94970200	8.37007500	15.41309100
C	1.55910500	8.42894800	12.63334000
C	7.88863200	11.32176500	14.94699500
C	-0.28288900	9.74624000	11.73825600
H	-0.85762400	10.67078700	11.74173200
C	2.43102200	7.49873600	14.62546200
C	8.20898700	7.40495900	17.29050800
C	0.23668000	10.47261800	14.93360100
C	5.90048100	6.70255500	16.90205900
C	5.87153100	7.53727500	15.79994100
C	1.04379200	10.69630000	13.66332100
H	2.09894100	10.59724300	13.95378300
C	1.17193600	7.03059100	15.05694800
H	0.30801400	7.32054300	14.47035100
C	0.89000900	12.09029400	13.06568800
C	8.91908200	12.24004700	14.77597600
H	8.95567100	13.11870400	15.41814500
C	3.44461600	6.32082000	16.54268800
C	1.25986000	7.43231400	11.67080600
C	9.49445000	7.27916500	18.11912300
C	9.84696600	10.92592700	13.01692600
H	10.60174700	10.77673500	12.24756600
C	9.90739600	12.06865800	13.80414500
C	-0.60887800	8.74977600	10.82151500
C	8.84690900	9.96222100	13.18328500
C	1.02551600	6.23979200	16.19489500
C	1.62287000	12.40316300	11.91312800
H	2.24897600	11.63753400	11.45723800
C	-1.15974100	10.40552700	14.91071600
H	-1.68828500	10.49142700	13.96502300
C	0.18634400	7.60597200	10.79744900
H	-0.00908900	6.84796900	10.04118200
C	0.88775600	10.33200300	16.15982400
H	1.97433000	10.33852000	16.18892700
C	-0.34827500	5.76342000	16.68535700
C	3.53624700	7.13105800	15.42692500
C	2.16724900	5.87959600	16.91862200
H	2.06790600	5.23572100	17.78481800
C	2.51359200	5.86986300	10.11233900
C	7.09226500	6.64060300	17.63982400
H	7.14688000	5.97323300	18.49247900
C	6.79479200	11.59544600	15.96879400
H	6.37276600	10.62808400	16.26016400
C	9.87982200	7.69210800	12.97019900
C	0.09784000	13.08698000	13.63489500
H	-0.46924800	12.87783200	14.53690300

C	5.65157700	12.41035200	15.38413500
C	8.89732300	8.68440600	12.36138500
H	7.90555000	8.21966900	12.46183100
C	2.14203300	6.19999600	11.55921200
H	3.07717600	6.47045600	12.06702800
C	1.56097400	13.66983600	11.34654000
H	2.14379300	13.89299100	10.45682300
C	1.60573500	4.98161700	12.29729600
C	0.02744600	14.35857200	13.06336900
H	-0.59870900	15.11822800	13.52401000
C	4.69507900	5.84374400	17.27700900
C	-1.88441600	10.23475600	16.08620800
H	-2.96963400	10.18915500	16.04787600
C	11.26200300	7.90038500	12.91349400
H	11.65608200	8.77684400	12.40656300
C	5.86308400	13.46692700	14.49557500
H	6.86712400	13.67379100	14.13521100
C	0.16743600	10.15899800	17.33944100
H	0.69623700	10.04717500	18.28236200
C	7.35405600	12.22305600	17.24232300
C	-1.49038600	6.24961100	15.78528300
H	-1.53477600	7.34394900	15.74636400
H	-2.44514800	5.88758100	16.18302700
H	-1.38708300	5.87062700	14.76162700
C	2.69129600	4.55312700	9.67654400
H	2.51637300	3.73040500	10.36352700
C	9.97815100	5.81610100	18.10700500
H	9.22769000	5.13999100	18.52815700
H	10.89471200	5.71866900	18.70142100
H	10.19577200	5.49125800	17.08370900
C	-1.22340000	10.11688000	17.30755600
H	-1.78909800	9.98030900	18.22518400
C	12.14364200	6.98812600	13.48401900
H	13.21409900	7.16780200	13.42947700
C	-0.59514400	6.30171100	18.10828100
H	0.15695200	5.93114500	18.81243000
H	-1.58224500	5.98464100	18.46712600
H	-0.56052300	7.39654900	18.11694600
C	0.75614100	14.65629800	11.91758800
H	0.70386800	15.64666900	11.47380500
C	4.34749500	12.15706100	15.82174300
H	4.17264200	11.33819300	16.51775700
C	10.63097200	8.15565100	17.57683200
H	10.88973000	7.88680200	16.54584200
H	11.52423900	8.01371700	18.19521900
H	10.37377200	9.22076500	17.60143500
C	-1.77772900	8.90376600	9.88557800
H	-2.69642900	8.50890400	10.33781300
H	-1.61255100	8.35724700	8.95198100
H	-1.95841800	9.95615600	9.64597600
C	0.32484300	4.48126000	12.05316600
H	-0.34061000	5.00825600	11.37513500
C	10.98302500	13.10269600	13.60748700
H	10.59759200	13.97261600	13.06087000
H	11.82255600	12.69706500	13.03556000
H	11.36147600	13.46717500	14.56823200
C	4.80164900	14.26289900	14.07033100
H	4.98652800	15.08144600	13.37894900
C	9.21085400	7.69737500	19.57495500
H	8.84870500	8.73042500	19.61951400
H	10.12707700	7.62761400	20.17382400
H	8.45423400	7.05399700	20.03535200
C	2.74987400	6.90237000	9.19690400
H	2.61726900	7.93396300	9.51334500
C	9.11328300	8.92183200	10.87094100
C	3.28608200	12.95112300	15.39798500
H	2.27842200	12.74173800	15.74600900
C	3.51000300	14.01067200	14.52221200
H	2.67694500	14.61804000	14.18006500
C	9.70496200	7.94599500	10.06280900
H	10.10292400	7.04266200	10.51653000
C	-0.38776500	4.22443900	16.71992100
H	-0.22009600	3.81491700	15.71853200
H	-1.36615100	3.87981400	17.07697900
H	0.37853600	3.81569500	17.38666900
C	9.40686000	6.54800900	13.61327600
H	8.33545600	6.38325000	13.68881600
C	9.78612900	8.11111100	8.68195800
H	10.24884300	7.33661700	8.07586800
C	-0.10694600	3.30470400	12.65956600
H	-1.10673600	2.92974400	12.45661100
C	7.22253700	13.57795400	17.54939300
H	6.67047300	14.23304500	16.88128800
C	11.65898200	5.84372300	14.11708600
H	12.34803200	5.12918700	14.55910500
C	4.69750800	12.24226100	8.96450000
H	4.97669600	12.38168100	7.91649100
H	3.66967400	12.59540600	9.10367700
C	3.13821200	6.63062900	7.88962500
H	3.31394900	7.45232000	7.19969800
C	2.43524800	4.28609800	13.17949100
H	3.42360700	4.68011700	13.40552500
C	5.39749100	12.18784800	11.23552100
H	6.27856200	12.12626900	11.88577700
H	4.56633300	12.62133400	11.80741900
C	8.05727400	11.40182500	18.13116200
H	8.15597300	10.34275100	17.90090300
C	3.07843000	4.27702300	8.36571400
H	3.20298800	3.24422700	8.05101400
C	3.30124300	5.31314300	7.46434200
H	3.59835400	5.09855600	6.44148400
C	0.73839800	2.60613800	13.51923600
H	0.40186500	1.68662300	13.99043000
C	2.01043400	3.10650400	13.78471900
H	2.67229300	2.58242600	14.46945800
C	10.28635600	5.62545900	14.17645400
H	9.89382900	4.73854400	14.66660700
C	5.64709300	12.94802700	9.93936700
H	5.43976600	14.01644800	10.04529300
H	6.68684300	12.82374700	9.61546600
C	7.79212100	14.10294700	18.70989900
H	7.67965200	15.16116600	18.93081700
C	4.97653200	4.38235500	16.85328700
H	5.86579800	4.00079400	17.36755100
H	5.14695400	4.32341300	15.77238700
H	4.12212500	3.74363900	17.10378100
C	8.62554900	11.92229200	19.28804700
H	9.16781600	11.26724200	19.96532800

C	8.49767000	13.28007900	19.58187800
H	8.93937300	13.68927000	20.48628500
C	9.27746300	9.25840500	8.07948600
H	9.34279100	9.38915000	7.00291500
C	4.46962000	5.88995800	18.80065100
H	3.62499300	5.26031900	19.09102400
H	4.26928300	6.91474200	19.13067200
H	5.34520600	5.51677300	19.33775500
C	4.82187300	10.79045000	9.40157000
H	3.92784700	10.18870000	9.20603500
H	5.69338700	10.30814800	8.93679200
C	8.60656500	10.07198800	10.25314700
H	8.13570100	10.84031800	10.86011100
C	8.68779000	10.23959700	8.87404300
H	8.28665500	11.14087100	8.41751900
O	5.53688100	7.29380500	11.49443000
C	5.96911600	7.51078100	10.10621800
C	5.85985800	5.92522800	11.88568200
C	6.46332100	6.15714400	9.61786800
H	5.11283800	7.88487300	9.54173200
H	6.76630000	8.25998100	10.11959200
C	6.93692300	5.48764500	10.91187000
H	6.16480000	5.94037700	12.93757800
H	4.96051400	5.30607500	11.77280500
H	7.25914000	6.26582400	8.87612500
H	5.63782300	5.58801100	9.17547300
H	7.91467900	5.87824900	11.21632500
H	6.99811900	4.39876700	10.83451700

TS_CaTHF_r

Final Single point energy: -4539.456976368901

Ca	0.34634300	3.70969500	4.70777500
O	-0.07533000	5.08738800	2.88891900
O	0.73776600	1.43138100	5.31586800
N	-1.78601900	4.55473700	4.86546800
N	2.25608500	4.86577000	4.16438700
C	-2.17856100	5.47956100	3.91604300
C	-1.29798800	5.77446300	2.86150100
C	2.14837800	8.11411400	5.21119400
C	2.22966900	5.63096700	3.01444500
C	-4.76950300	2.85788700	7.37444100
C	-2.89844500	4.38857000	7.05411200
C	-1.57119300	6.65513800	1.83196600
C	3.43335800	6.04511200	5.95594300
C	2.21311500	6.93205200	6.15981600
H	1.33957500	6.31140200	5.90557300
C	-2.78848600	4.01548300	5.69472700
C	3.33033700	6.31510600	2.45754900
H	4.28547700	6.21168500	2.95858600
C	-3.87863100	3.81064600	7.86180100
H	-3.94115700	4.11040600	8.90629200
C	-3.39636300	6.19002000	3.90858100
H	-4.09136700	5.99058500	4.71605600
C	-3.69447700	7.13571800	2.92759700
C	3.20737500	7.11183900	1.32124000
C	1.01374600	5.77323000	2.32692700
C	2.03079300	7.33120000	7.62067300
C	-2.47961000	6.86258600	7.42570400
C	0.82790200	6.59972700	1.23503400
C	4.48905700	4.13032000	4.90068500
C	3.39617600	5.01743500	4.98024800
C	3.23634000	8.97163500	5.03847700
H	4.17494500	8.75576600	5.54360300
C	5.17685400	3.19524000	2.65068500
C	4.56991200	6.21662900	6.74084000
H	4.57685000	7.00396500	7.49253100
C	0.95932800	8.39092600	4.53668400
H	0.11006900	7.71844800	4.64447100
C	-2.77958700	7.35564200	1.88730800
H	-3.00839700	8.07865500	1.11420100
C	-4.96890800	7.98732100	2.99396400
C	1.94678700	7.26407400	0.72583700
H	1.83499000	7.90829700	-0.13820800
C	-0.58338300	6.71725100	0.66509400
C	-4.62176200	2.44992400	6.05024400
H	-5.25708000	1.65274500	5.66731900
C	2.01591100	8.65490900	8.05886900
H	2.16680700	9.46078900	7.34720800
C	-3.65369000	2.99997800	5.21209200
C	1.56858700	7.94010300	10.32421700
H	1.37849100	8.17535900	11.36767800
C	-1.97094000	5.44506700	7.63434600
H	-1.02706600	5.38618900	7.07230000
C	1.80982300	6.31704000	8.55985700
H	1.81082500	5.27891300	8.23063100
C	4.75795400	1.61759100	4.60895500
C	-3.83556700	7.18618300	7.48864700
H	-4.57084500	6.39838400	7.63093500
C	-1.62840400	5.15162100	9.09019200
C	5.61024200	4.33078000	5.70888400
H	6.43731300	3.62615700	5.65249900
C	1.78942800	8.95639400	9.40228000
H	1.77621800	9.99478100	9.72238900
C	-1.55393800	7.88717900	7.22262900
H	-0.49450300	7.64872500	7.18241800
C	6.56713700	3.33613600	2.62227900
H	7.13745300	3.26454900	3.54392500
C	4.42234500	2.94948000	3.94815400
H	3.36307100	2.88036200	3.65641600
C	-5.85112100	2.28220000	8.24814900
H	-5.57794600	2.33640400	9.30617800
H	-6.05191000	1.23636000	7.99491300
H	-6.79152300	2.83373700	8.12281500
C	-2.00745400	5.97987800	10.14453800
H	-2.55728700	6.89367500	9.93939700
C	0.84968200	9.50880700	3.71512700
H	-0.08155500	9.69376000	3.18561200
C	5.68383900	5.38492300	6.61400300
C	-0.90790700	3.98888500	9.38493500
H	-0.61029000	3.33218500	8.56933200
C	-5.67961900	8.02201100	1.62880400
H	-6.59629600	8.61942200	1.70256200
H	-5.95098100	7.01020100	1.31031100
H	-5.05672600	8.47022000	0.84902000
C	-0.57945100	3.65698900	10.69221600
H	-0.01686000	2.74970000	10.89660000
C	-3.49151200	2.47052100	3.79575500
H	-2.45500300	2.69941400	3.50428000

C	4.16740400	9.33199600	0.61582500
H	4.00876500	9.74590800	1.61627900
H	3.28507200	9.56658100	0.01203400
H	5.03062500	9.83429800	0.16236500
C	1.57851800	6.61325400	9.89556600
H	1.38115500	5.81004100	10.59969900
C	-0.84625900	5.48996600	-0.24276700
H	-1.87100800	5.52112400	-0.63005800
H	-0.71604000	4.55775000	0.31594300
H	-0.14530100	5.48862600	-1.08537000
C	4.41873100	7.81465700	0.69392900
C	1.93088900	10.37246700	3.56719000
H	1.85009000	11.24559600	2.92551200
C	3.12593100	10.09856500	4.23048200
H	3.97906100	10.76126900	4.11076800
C	-3.32109300	9.52469000	7.16176000
H	-3.65010200	10.55468800	7.05482800
C	7.23386000	3.55819700	1.42187700
H	8.31486600	3.66884400	1.41884800
C	4.47349700	3.27801500	1.44864800
H	3.38973200	3.18654100	1.45859500
C	-1.68199500	5.65009400	11.46057400
H	-1.98764200	6.30955800	12.26842100
C	-0.97027100	4.48976800	11.74154100
H	-0.71677800	4.23491700	12.76676300
C	-4.56937800	9.42218600	3.39185400
H	-3.89511800	9.86302100	2.64961700
H	-4.05573800	9.42149900	4.35972900
H	-5.45906600	10.05985900	3.47103900
C	-1.96706200	9.20785600	7.08454000
H	-1.22817400	9.98699200	6.91546100
C	-4.25225000	8.50960100	7.36521600
H	-5.31145000	8.74726000	7.41874400
C	4.47026600	1.40316000	5.96225700
H	4.11391100	2.23208600	6.56798500
C	-0.76183300	7.98693300	-0.16783800
H	-0.06965900	7.99288300	-1.01448800
H	-0.58953700	8.88699600	0.43172500
H	-1.77265500	8.03065700	-0.58338400
C	0.80652100	0.86820600	6.65169300
H	0.05276100	1.37832900	7.25867100
H	1.80685900	1.05893400	7.06028400
C	6.52124000	3.63695900	0.22658400
H	7.04241500	3.81223000	-0.71043900
C	5.70590600	7.58491300	1.49519300
H	5.96915800	6.52196300	1.54363200
H	5.61580200	7.96661600	2.51887700
H	6.53490900	8.11272200	1.01055800
C	6.91713100	5.61694400	7.44481500
H	6.65888400	5.95542000	8.45331500
H	7.55149900	6.39079500	6.99467000
H	7.51797500	4.70651200	7.52866700
C	5.13774700	3.49246800	0.24365100
H	4.56969400	3.55480400	-0.68049400
C	4.63522000	7.26781500	-0.73038300
H	5.50460300	7.75015400	-1.19428400
H	3.76336800	7.45342700	-1.36594700
H	4.81485700	6.18775100	-0.70259300
C	-4.37131200	3.16321000	2.76875000
C	-3.63150000	0.94944400	3.74857600
C	-5.96958600	7.45629600	4.02817600
H	-6.87625400	8.07161100	4.00758700
H	-5.56317300	7.49851200	5.04337300
H	-6.25380000	6.42059100	3.80974800
C	-4.65096000	4.00765900	0.51387800
H	-4.22628500	4.23160400	-0.46087400
C	4.63599200	0.14802400	6.54047700
H	4.41192600	0.00790800	7.59507300
C	5.22090800	0.53538400	3.85378200
H	5.44883000	0.67734100	2.80103100
C	1.31779000	0.43477800	4.42497700
H	2.40883300	0.53870900	4.44582500
H	0.94246300	0.64207100	3.41808500
C	5.09243000	-0.92349700	5.77636100
H	5.22613000	-1.90291300	6.22716600
C	-2.82402300	0.17428000	4.59128000
H	-2.13317300	0.67490000	5.26811600
C	0.86908400	-0.91384200	4.98658600
H	-0.01810800	-1.27421500	4.46071000
H	1.66252000	-1.65684300	4.87357700
C	5.38529900	-0.72190300	4.43034900
H	5.74650600	-1.54699600	3.82234600
C	-5.71149200	3.45615300	3.02372000
H	-6.12751900	3.25387200	4.00682700
C	-3.85115500	3.44918300	1.50560500
H	-2.80297000	3.24079900	1.30166200
C	-5.99153300	4.28193700	0.77211900
H	-6.61983000	4.71606800	-0.00067900
C	-6.51731200	4.00846800	2.03213900
H	-7.55911200	4.23166400	2.24666800
C	-2.91463200	-1.21174800	4.59310300
H	-2.29126800	-1.79608500	5.26514500
C	0.54392400	-0.62911400	6.47462200
H	-0.50043400	-0.86577100	6.69425100
H	1.17287400	-1.21199000	7.15231200
C	-4.52104100	0.29327800	2.89818000
H	-5.15500800	0.87062400	2.23224000
C	-3.81269300	-1.85772400	3.74342300
H	-3.88777500	-2.94142000	3.74668400
C	-4.61089000	-1.09929400	2.89591500
H	-5.31440600	-1.58842900	2.22759500

TS_F_THFCaBr

Final Single point energy: -7213.828717333734

Ca	0.29165000	4.41792900	5.42642000
Br	0.89274000	3.08718700	7.90880100
O	-0.11509800	6.64263900	4.62306200
O	-0.93036500	4.27385200	2.58381300
N	-1.90266400	5.27218100	5.94982900
N	2.28175700	5.70824500	5.12510700
C	-2.35683500	6.34352100	5.23652800
C	-1.41443000	7.10671300	4.49601500
C	3.26152500	8.95528100	6.66043600
C	2.19690000	6.80937600	4.31462500
C	-4.62376600	3.09639500	8.37451100
C	-2.90003600	4.80144100	8.13197800
C	-1.73982900	8.22299700	3.75191400
C	3.81271700	6.45422000	6.88417600

C	2.87478200	7.60157600	7.22793800
H	1.90931200	7.34185800	6.77236300
C	-2.83198100	4.56813500	6.73271200
C	3.29148700	7.46767100	3.71713200
H	4.27654900	7.07247000	3.93598700
C	-3.80627600	4.09183200	8.91288100
H	-3.85056000	4.28914100	9.98218400
C	-3.69125900	6.80498500	5.18712900
H	-4.42524800	6.25343100	5.76267200
C	-4.06226000	7.92905700	4.44966400
C	3.12595700	8.55178600	2.85603200
C	0.91621800	7.33689500	4.01593100
C	2.61634900	7.67936400	8.73320700
C	-2.34135400	7.25074600	8.41373300
C	0.70994000	8.44597700	3.21922300
C	4.27662900	4.39469700	5.68110700
C	3.46328300	5.54093100	5.85423400
C	4.58541300	9.38690800	6.57071200
H	5.38931000	8.70083100	6.82280100
C	4.10489700	3.82890500	3.21852000
C	4.95792800	6.24335200	7.64979200
H	5.17328200	6.92826500	8.46964800
C	2.24605000	9.84523600	6.30157200
H	1.21329600	9.50577200	6.34059500
C	-3.08670400	8.61999500	3.72681400
H	-3.36228100	9.49585900	3.14824600
C	-5.51312900	8.42911500	4.40429100
C	1.83568200	9.03805700	2.62508500
H	1.68843500	9.89157800	1.97159900
C	-0.67922400	9.04802800	3.02713300
C	-4.50791500	2.82470000	7.01699600
H	-5.08363000	2.00554700	6.58926300
C	2.93548700	8.79318900	9.51062800
H	3.40514500	9.65704900	9.04902500
C	-3.65220100	3.55460800	6.18737700
C	2.03383100	7.72322300	11.48164300
H	1.79680100	7.74122800	12.54240000
C	-1.95385700	5.82427400	8.75039700
H	-0.97699400	5.64054900	8.27828800
C	2.00230100	6.58395400	9.35360800
H	1.74859700	5.70322600	8.76426700
C	4.49798100	1.99621200	4.91026500
C	-3.65875400	7.68970600	8.55625100
H	-4.42450200	6.97731200	8.85565300
C	-1.73599900	5.62216800	10.24680800
C	5.42232700	4.22992400	6.45751800
H	6.03239100	3.34145400	6.30863700
C	2.64911600	8.81337600	10.87701200
H	2.90440000	9.69214900	11.46442800
C	-1.36968600	8.16699600	8.01069900
H	-0.34084800	7.83212200	7.89496800
C	5.23380000	4.56075300	2.84685600
H	5.95252700	4.85394700	3.60964700
C	3.87471700	3.35773500	4.64246300
H	2.79173000	3.18635700	4.72499000
C	-5.56461700	2.31715800	9.25554600
H	-5.01815200	1.76614400	10.03059900
H	-6.14253700	1.59352600	8.67262100
H	-6.27085300	2.98065500	9.76935800
C	-1.97080600	6.62009200	11.19293200
H	-2.34858200	7.58684900	10.87451800
C	2.53816900	11.13825500	5.88424900
H	1.73090800	11.80806000	5.59853600
C	5.79565300	5.15150300	7.43518100
C	-1.22400100	4.39511800	10.69014800
H	-1.00698500	3.62053700	9.95927100
C	-6.04928200	8.30475300	2.96561400
H	-7.09071300	8.64960900	2.91204700
H	-6.01228900	7.26150000	2.63537500
H	-5.45413600	8.90310700	2.26746800
C	-0.96301000	4.17404500	12.03595200
H	-0.55465000	3.21709600	12.35118000
C	-3.57591200	3.22896300	4.70291700
H	-2.66474800	3.71065400	4.32759100
C	4.27896700	10.70161500	2.16129600
H	4.32502100	11.04362900	3.20025800
H	3.37207400	11.11339400	1.70777000
H	5.13870200	11.11573500	1.61908700
C	1.71083700	6.60593100	10.71107400
H	1.21456200	5.75249600	11.16468200
C	-1.01533500	9.13323800	1.52183000
H	-2.01681700	9.54893400	1.37056600
H	-0.98326800	8.14065200	1.06127200
H	-0.29838600	9.77501700	0.99903700
C	4.31152500	9.16372500	2.09746700
C	3.86252400	11.56751800	5.81991100
H	4.09661300	12.57732700	5.49272700
C	4.88411200	10.68258500	6.15528100
H	5.92197700	11.00013000	6.08863000
C	-3.01991300	9.92533700	7.91056900
H	-3.28321600	10.96006000	7.70706000
C	5.43974200	4.91983300	1.51618300
H	6.32590100	5.48602700	1.23914100
C	3.17255100	3.47654600	2.23870600
H	2.28815700	2.92032600	2.55521900
C	-1.70892800	6.39982900	12.54609200
H	-1.89332000	7.19644700	13.26275900
C	-1.20576100	5.17731100	12.97525800
H	-0.99619900	5.00700800	14.02825700
C	-5.57609800	9.90643900	4.83752500
H	-4.98827600	10.54884300	4.17448900
H	-5.18546200	10.02410200	5.85384100
H	-6.61494600	10.26097000	4.81963800
C	-1.70473700	9.49362900	7.75556200
H	-0.93658900	10.19236400	7.43393300
C	-3.99594900	9.01796400	8.31629400
H	-5.02703900	9.34328500	8.43173800
C	3.93320400	1.20066300	5.91418100
H	3.05577400	1.56654900	6.44455500
C	-0.67929400	10.47831600	3.61745100
H	0.09748700	11.09112600	3.14779200
H	-0.48284700	10.43692500	4.69375100
H	-1.64842300	10.96488700	3.46429900
C	-0.93641000	3.01790200	1.87228900
H	-1.72304700	2.39753300	2.31026300
H	0.02408100	2.51487900	2.03732000
C	4.50568500	4.56983600	0.54415300
H	4.65851200	4.86258500	-0.49171100

C	5.66220600	8.70190300	2.66010700
H	5.79557700	7.62130600	2.55081400
H	5.75715300	8.95542200	3.72216000
H	6.47436700	9.19671000	2.11405600
C	7.04995600	4.96224500	8.24756900
H	7.88610300	5.54447100	7.83735500
H	7.35663500	3.91159500	8.26132200
H	6.90440500	5.29015400	9.28277200
C	3.36836200	3.85208800	0.91281800
H	2.62635000	3.58610500	0.16283500
C	4.22173400	8.72135200	0.62286400
H	5.06261200	9.12831300	0.04527600
H	3.28801900	9.07064500	0.16850400
H	4.24507900	7.62802500	0.55050000
C	-4.72026500	3.78284000	3.86548900
C	-3.40427700	1.72513500	4.49191900
C	-6.43567100	7.62930000	5.33214300
H	-7.45191000	8.03831400	5.27891100
H	-6.09844000	7.68680100	6.37331400
H	-6.48121100	6.57458700	5.04195900
C	-5.46977900	4.59890500	1.70487500
H	-5.23179200	4.91727500	0.69281600
C	4.47649100	-0.03919800	6.22760800
H	4.01824700	-0.64306100	7.00678800
C	5.61039700	1.51181600	4.22104100
H	6.05066400	2.10842200	3.42649400
C	-0.26292800	5.19246500	1.70858900
H	0.82451300	5.01757500	1.74222700
H	-0.47317600	6.20198100	2.06371200
C	5.59548900	-0.51189600	5.54113900
H	6.01783400	-1.48394100	5.78338900
C	-2.13586600	1.16148400	4.66896800
H	-1.26528200	1.78446800	4.87209600
C	-0.82938000	4.89111200	0.31993500
H	-1.73060400	5.48878700	0.14523800
H	-0.10916500	5.12378100	-0.47086100
C	6.15781300	0.26767000	4.53526700
H	7.02435900	-0.09276000	3.98593600
C	-6.04085700	3.84079400	4.31505300
H	-6.27056200	3.56959000	5.34142600
C	-4.44905500	4.18566500	2.55344100
H	-3.41755800	4.19604300	2.20959900
C	-6.78940100	4.62017000	2.15331400
H	-7.58914300	4.94593900	1.49322800
C	-7.06715000	4.25045400	3.46550800
H	-8.08832700	4.28736700	3.83710100
C	-1.93821100	-0.20680400	4.52588100
H	-0.93698900	-0.60929300	4.65336000
C	-1.17754800	3.38373600	0.39563000
H	-2.21908000	3.20923600	0.10663700
H	-0.54255600	2.78075700	-0.26098000
C	-4.46698100	0.88238100	4.15785400
H	-5.45530500	1.30253800	3.99049500
C	-3.00853900	-1.04324800	4.21279900
H	-2.85459800	-2.11361200	4.10204900
C	-4.27269200	-0.49200700	4.02538600
H	-5.11418000	-1.13048600	3.76715600
F	0.91866200	2.13409800	4.12096800

TS_FCaBr_THF

Final Single point energy: -7213.833224409868

Ca	11.11866300	15.82684200	6.21692200
O	11.65790900	17.23598600	4.37848600
F	10.15087100	17.73014200	7.12424000
N	13.44059400	16.42971300	6.10614600
N	9.64895200	15.54967500	4.32469000
C	14.43971300	15.93275800	6.94934600
C	14.98133900	18.23803600	5.40114300
H	15.73670800	17.88075500	6.09105400
C	12.80276700	18.00760600	4.42761400
C	10.65413100	17.55937400	3.48945100
C	8.95577200	14.39849600	3.95970700
C	13.76232100	17.52514900	5.35486400
C	15.21513600	19.36243700	4.60944300
C	14.53859200	16.35558400	8.29383600
C	14.21213000	19.80337400	3.74178300
H	14.37341900	20.68783600	3.13383900
C	10.70764100	18.66916500	2.67007900
C	7.88453600	13.91399400	4.74776600
C	13.73551400	18.74123200	8.62495400
C	12.98856700	19.12191900	3.63568100
C	14.93688700	19.33159000	9.02249400
H	15.71217300	18.71728800	9.47516700
C	9.59820800	16.61427700	3.46413700
C	8.55730000	16.87159800	2.54839500
H	7.74240000	16.15652600	2.51970200
C	8.54711000	18.00589300	1.73713400
C	13.12434100	16.93084100	10.30922500
C	12.75671600	19.53063500	8.01795200
H	11.82889300	19.06255900	7.68334700
C	7.22201600	12.74341200	4.38691300
H	6.39567400	12.39229300	5.00242200
C	6.69016500	15.96166200	5.55936500
C	7.45007200	12.76171300	7.53699300
H	8.44643700	12.53618300	7.16141800
C	13.46041600	17.26772900	8.86086500
H	12.54705400	17.05908700	8.28600400
C	15.32604200	14.92353100	6.50212700
C	14.16491900	21.48162500	8.24504400
H	14.33297300	22.54508100	8.09387200
C	15.51582000	12.82556100	5.09615900
C	15.60173700	15.10245800	3.98692900
C	6.77179600	13.87967100	7.03143200
C	7.60824300	11.98963500	3.27852100
C	15.06986900	14.28218600	5.14487500
H	13.97431200	14.27307900	5.03716400
C	12.97508000	20.89274300	7.82516000
H	12.21138300	21.49373400	7.33792000
C	16.54676700	15.01437300	8.60783900
C	7.46491200	14.72249400	5.96906300
H	8.39118500	15.08467600	6.43707700
C	15.14912400	20.69478700	8.84143400
H	16.08896200	21.14268400	9.15568200
C	15.59283300	15.90798800	9.09035100
H	15.65166000	16.24158600	10.12538600
C	9.62546500	18.89230100	1.80404100
H	9.63402200	19.78037800	1.17992900
C	5.51360900	14.18190100	7.55244900

H	4.97792700	15.05433700	7.19081200
C	16.37162600	14.50341100	7.32135600
H	17.04744500	13.72912500	6.96163900
C	10.63194200	14.01267700	2.09558800
H	11.14973400	14.73091300	2.74639200
C	9.37945000	13.60938300	2.85784700
C	11.90413900	19.61642300	2.68270900
C	8.71193200	12.42640900	2.54739800
H	9.09125700	11.80611400	1.73540300
C	13.04423500	17.89378700	11.31555600
H	13.25500800	18.93273700	11.08044800
C	12.82641000	15.60057800	10.63601900
H	12.86142100	14.84151000	9.85761800
C	16.54178800	20.13348700	4.66691700
C	16.38052100	12.32039200	4.12556900
H	16.78470800	12.98375700	3.36678600
C	17.53521500	19.50965900	5.65486200
H	17.77740800	18.47682700	5.37947600
H	17.13447400	19.50828700	6.67477800
H	18.46581500	20.09000200	5.65536500
C	16.91138400	15.58603400	3.98430200
H	17.54487400	15.40656800	4.85029700
C	14.79104500	15.35545100	2.88043200
H	13.76685200	14.98749900	2.87722600
C	10.39359300	14.72529800	0.77699000
C	7.35752700	18.33742100	0.82607300
C	12.69053200	17.53940500	12.61827100
H	12.63307800	18.30790000	13.38519300
C	11.58810900	12.83200000	1.93476700
C	7.11908200	17.22593800	5.96495000
H	8.04807500	17.33111600	6.52765600
C	5.54261000	15.85557000	4.76866800
H	5.22346000	14.87446200	4.42271000
C	9.36318100	14.37285800	-0.09587700
H	8.63717700	13.62450800	0.20949300
C	6.87403100	11.95838000	8.51160500
H	7.42009600	11.09648900	8.88714400
C	12.40987600	16.21523200	12.93449900
H	12.13485400	15.93745600	13.94872700
C	14.99197400	11.93888100	6.04687500
H	14.28875800	12.31353200	6.78681400
C	17.71239100	14.58569100	9.46028000
H	17.46488600	14.64044900	10.52547200
H	18.58613700	15.22968300	9.29358300
H	18.01579400	13.55899700	9.22992000
C	12.47789900	15.24629900	11.93253100
H	12.25081800	14.20855800	12.16240400
C	5.60874000	12.26056900	9.01709100
H	5.15890200	11.63398900	9.78310000
C	11.94867800	12.29853300	0.69709700
H	11.53899800	12.72512700	-0.21418600
C	17.40471200	16.29531000	2.89426400
H	18.42694100	16.66567400	2.90858500
C	16.72146900	10.96699600	4.10640400
H	17.39216200	10.59534000	3.33553900
C	4.93643300	13.37923500	8.53852700
H	3.95603900	13.63668100	8.93187400
C	4.81299800	16.98771400	4.41960900
H	3.91957100	16.88850300	3.80772200
C	5.23748900	18.24738500	4.83971500
H	4.67628700	19.13504300	4.55860900
C	11.43814000	21.01801600	3.13710800
H	12.27745100	21.72207700	3.14055700
H	11.02693500	20.96499100	4.15049200
H	10.66253900	21.40631500	2.46766500
C	6.36263200	17.17392400	0.72339700
H	5.91278300	16.94195800	1.69453100
H	6.85089300	16.26833200	0.34500000
H	5.55413200	17.44279400	0.03286400
C	12.14153600	12.27233700	3.09353600
H	11.86706300	12.67267300	4.06953500
C	15.27478400	16.07937600	1.79429700
H	14.62456300	16.27944400	0.94642000
C	6.39758000	18.36145500	5.60140600
H	6.75605400	19.34089800	5.90773100
C	16.58575400	16.54849200	1.79536100
H	16.96325800	17.11868100	0.95052100
C	12.48635900	19.70988400	1.25429200
H	11.72819500	20.05696500	0.54487700
H	12.83782900	18.72475400	0.92871200
H	13.33132800	20.40515500	1.21940100
C	6.61764600	19.55819700	1.40686000
H	5.74913600	19.81730000	0.78609200
H	7.27900600	20.43005900	1.45607600
H	6.26880000	19.34085000	2.42222200
C	17.19755100	20.14544300	3.27274700
H	18.15286900	20.68629800	3.30479600
H	16.55476100	20.63397700	2.53312600
H	17.38552300	19.12294000	2.92982800
C	16.28031300	21.58637700	5.10658000
H	15.80914200	21.60363400	6.09422400
H	15.61448800	22.10168400	4.40655500
H	17.22338200	22.14708100	5.15702800
C	16.20147300	10.09709800	5.05780100
H	16.46257700	9.04199700	5.04012100
C	6.86614200	10.73607600	2.89528200
H	7.52970300	10.02093500	2.39755100
H	6.04153500	10.95272300	2.20268100
H	6.43347200	10.24710400	3.77437700
C	11.29618200	15.71419400	0.37632500
H	12.08179800	16.01922600	1.06450000
C	12.84064600	11.22750300	0.61685800
H	13.11125500	10.82758400	-0.35750700
C	7.83865700	18.67233900	-0.59741700
H	8.39173800	17.82834200	-1.02197300
H	8.49468600	19.54843900	-0.61210300
H	6.97833500	18.88789400	-1.24435500
C	15.33005900	10.59237900	6.02929600
H	14.89959000	9.92296700	6.76991200
C	13.03372000	11.21112900	3.01405900
H	13.46689700	10.80687400	3.92484200
C	13.38802800	10.68197400	1.77256800
H	14.09410800	9.85755800	1.71303400
C	9.25484400	14.97350400	-1.34809400
H	8.44371800	14.68783600	-2.01359200
C	11.19103900	16.31836300	-0.87110300
H	11.89743500	17.09399800	-1.15615500
C	10.17432500	15.94032300	-1.74629400

H	10.08691400	16.41235100	-2.72152400
Br	11.45842000	13.06713100	6.96722900
O	9.96633500	14.41911100	9.17474000
C	9.94508400	13.26044800	10.02423300
C	9.25288000	15.47957300	9.83160100
H	10.95230400	13.07408300	10.42313200
H	9.66453800	12.40404700	9.40216700
C	8.92427600	13.54463700	11.14445400
C	8.16450000	14.77484200	10.62913200
H	8.88625600	16.15830200	9.05394600
H	9.93077800	16.04046000	10.49841000
H	8.26740100	12.68799400	11.32721800
H	9.44227600	13.78772500	12.08010000
H	7.75468300	15.39404900	11.43408700
H	7.35019400	14.47280700	9.96154700

TS_F_(THF_r)CaBr

Final Single point energy: -7213.830922751797

Ca	0.34604800	3.57828100	4.53117100
Br	0.84321100	2.77064700	7.25053900
O	-0.03739300	5.70732400	3.54661800
O	0.49851100	1.24804400	4.02082400
N	-1.86024500	4.49480700	4.97460100
N	2.35098200	4.93797200	4.32079000
C	-2.29172400	5.46300900	4.10513600
C	-1.33147400	6.10325400	3.28219300
C	3.01249200	8.46698000	5.28403700
C	2.27789700	5.86491500	3.30757100
C	-4.93051300	3.02815000	7.49840200
C	-3.07633600	4.55842300	7.10045000
C	-1.64580400	7.03464400	2.31387600
C	3.72636700	6.10083400	5.98130200
C	2.69023800	7.20965800	6.07065900
H	1.77576700	6.78840800	5.62908600
C	-2.83599400	3.97582300	5.83429000
C	3.38830800	6.44213700	2.66027400
H	4.37037900	6.14018300	3.00726800
C	-4.12500200	4.09418900	7.89422000
H	-4.30088700	4.56150900	8.86195500
C	-3.62619800	5.89719700	3.94114400
H	-4.37811300	5.43853900	4.57236600
C	-3.98392200	6.85787100	2.99486900
C	3.24581900	7.32790100	1.59232200
C	1.00467600	6.26999000	2.84332500
C	2.34551300	7.52633400	7.52493900
C	-2.54140300	7.03907500	7.05984100
C	0.81643800	7.17795900	1.82072300
C	4.39480200	3.91001300	5.18285400
C	3.48881100	4.99497700	5.12217200
C	4.30425500	8.98855500	5.19721000
H	5.13468700	8.43122800	5.62146800
C	4.39554600	2.94642500	2.86536500
C	4.85108300	6.11914300	6.80376900
H	4.98023200	6.94925400	7.49813100
C	1.96472500	9.18494200	4.70182900
H	0.95969400	8.76949800	4.73148300
C	-2.99294600	7.40528200	2.17596300
H	-3.26236100	8.12831800	1.41288300
C	-5.43525500	7.32828300	2.82421100
C	1.95847700	7.68840900	1.18509500
H	1.82841400	8.36531000	0.34651000
C	-0.58096400	7.60137500	1.37972500
C	-4.61642700	2.38308800	6.30303500
H	-5.17695500	1.49415200	6.01569600
C	2.56356500	8.77269300	8.11263000
H	3.00599100	9.57424100	7.52784000
C	-3.57914100	2.82482900	5.48389800
C	1.62599200	7.99461800	10.19988300
H	1.33482000	8.17609700	11.23140800
C	-2.15727300	5.66965800	7.58600600
H	-1.17129300	5.43713900	7.15596300
C	1.76041500	6.51449200	8.29735000
H	1.58148600	5.53530600	7.85425200
C	4.70061200	1.40438900	4.88110200
C	-3.86050500	7.49320600	7.11198100
H	-4.63633600	6.82935900	7.48656700
C	-1.98427200	5.65149100	9.10165500
C	5.52730100	3.97930100	5.99000400
H	6.21475900	3.13535600	6.01022800
C	2.20969300	9.00418400	9.44320700
H	2.38564400	9.98371100	9.88142900
C	-1.55853900	7.89086500	6.55617900
H	-0.52888000	7.54259300	6.50891500
C	5.68455600	3.29821600	2.45532000
H	6.46974800	3.40388300	3.20147100
C	4.09470600	2.68646200	4.32950900
H	3.00664100	2.54584800	4.39108800
C	-6.05216700	2.53088000	8.37328700
H	-6.32645500	3.27864400	9.12368500
H	-5.76499700	1.61548000	8.90666500
H	-6.94383400	2.29474900	7.78188300
C	-2.22720400	6.75992000	9.91262600
H	-2.57076800	7.68808600	9.46592000
C	2.19411900	10.40264100	4.07100400
H	1.36562000	10.93716200	3.61332300
C	5.78651100	5.08543400	6.79931100
C	-1.51996600	4.47525400	9.70588200
H	-1.30220200	3.61238500	9.08176300
C	-5.91530400	7.04082500	1.38917000
H	-6.95402800	7.37389400	1.26023200
H	-5.86283300	5.96779200	1.17978500
H	-5.29852500	7.56003300	0.64839100
C	-1.30880500	4.41167800	11.07677500
H	-0.93525600	3.49139200	11.51887400
C	-3.20036700	2.06613600	4.22092200
H	-2.13394500	2.27923800	4.06528600
C	4.38831200	9.38871600	0.67540000
H	4.38858000	9.86201600	1.66266900
H	3.48389300	9.70943000	0.14898500
H	5.25486200	9.75668500	0.11036500
C	1.40119000	6.74636500	9.61839200
H	0.92630500	5.95448600	10.19124500
C	-0.83767100	7.05413700	-0.04379400
H	-1.83540400	7.34255700	-0.39434100
H	-0.77198400	5.96085900	-0.03629700
H	-0.09276700	7.44388500	-0.74727500
C	4.45760500	7.85738300	0.81390900
C	3.48353000	10.92729900	4.01213100

H	3.66676800	11.87682000	3.51580100
C	4.53890500	10.20906300	4.56858500
H	5.55280400	10.59757700	4.50887000
C	-3.20048600	9.61788700	6.17723200
H	-3.45739800	10.61330100	5.82439700
C	5.96822700	3.51498900	1.11041700
H	6.97745100	3.78293800	0.80692500
C	3.38441200	2.85760600	1.90798200
H	2.35330700	2.65667000	2.19828500
C	-2.01765700	6.69750900	11.29104400
H	-2.20801800	7.57709600	11.90119900
C	-1.55920900	5.52513200	11.88057700
H	-1.39005200	5.47775200	12.95335100
C	-5.51986900	8.84509300	3.08314800
H	-4.90025200	9.40465800	2.37466400
H	-5.16812700	9.07861900	4.09304300
H	-6.55650900	9.19298900	2.98093600
C	-1.88425800	9.16883500	6.11050900
H	-1.10724100	9.81511700	5.71009900
C	-4.18812600	8.77509100	6.68325600
H	-5.22092000	9.11203700	6.72899100
C	4.39558600	1.04259200	6.20141400
H	3.76692700	1.70216900	6.79650000
C	-0.67006200	9.14219500	1.36562300
H	0.08320200	9.57340800	0.69878800
H	-0.50389500	9.53673100	2.37397600
H	-1.65415600	9.47644800	1.02268200
C	1.43121000	0.30792300	4.60061500
H	1.64718900	0.64085700	5.61792300
H	2.35655000	0.31175800	4.00384900
C	4.95608400	3.40705500	0.15752400
H	5.17275400	3.58905900	-0.89211100
C	5.78587200	7.50798000	1.49771700
H	5.93727700	6.42467400	1.55340100
H	5.82659000	7.91461600	2.51490800
H	6.61681000	7.93557100	0.92358500
C	7.02560400	5.15183600	7.65346100
H	7.35076000	4.15213000	7.96021100
H	6.85099200	5.74693900	8.55607500
H	7.86177000	5.61610600	7.11326400
C	3.66177800	3.09310800	0.56335900
H	2.85176400	3.04462800	-0.15943800
C	4.45580700	7.22382000	-0.59097400
H	5.32358200	7.56589800	-1.17116700
H	3.54650700	7.48933600	-1.14101400
H	4.49522400	6.13219400	-0.51166700
C	-3.89911500	2.57824400	2.97458900
C	-3.30732400	0.55868600	4.41660800
C	-6.39473700	6.62469400	3.79238700
H	-7.41486200	6.99253400	3.62825700
H	-6.12683900	6.82090300	4.83683300
H	-6.39406500	5.54019100	3.63469200
C	-3.78035500	3.43378000	0.71767100
H	-3.17842100	3.77745400	-0.11995000
C	4.86382800	-0.14661300	6.74272500
H	4.60529600	-0.40788200	7.76572200
C	5.48172900	0.53410100	4.12103400
H	5.71490100	0.78333400	3.09029900
C	0.00509500	0.58069000	2.82609000
H	0.71958700	0.75709800	2.01413200
H	-0.93551800	1.05169100	2.54491600
C	5.65355600	-1.00599700	5.97687500
H	6.02059600	-1.93758300	6.39980300
C	-2.68987500	-0.01419200	5.53749600
H	-2.16477800	0.62958700	6.23998600
C	-0.10185500	-0.90727400	3.20217900
H	-1.14154800	-1.19772500	3.37446400
H	0.29847100	-1.53127600	2.39688300
C	5.95725500	-0.66039100	4.66532200
H	6.56354700	-1.32325100	4.05287100
C	-5.29365800	2.61001000	2.89387700
H	-5.88755600	2.30170000	3.75165000
C	-3.14284900	3.00768500	1.88152600
H	-2.04827400	3.04035400	1.93293300
C	-5.16963900	3.43375900	0.63008300
H	-5.66232400	3.76636600	-0.28042100
C	-5.92729400	3.02791500	1.72792700
H	-7.01355600	3.04529600	1.67857500
C	-2.74457900	-1.38323800	5.76256800
H	-2.25962300	-1.80237700	6.64055400
C	0.72799900	-1.03850800	4.49977700
H	0.07055200	-1.18291100	5.36206500
H	1.44626800	-1.86370200	4.46999500
C	-3.95561800	-0.28670800	3.51537600
H	-4.42488600	0.13219400	2.63030800
C	-3.40799200	-2.21836900	4.86302500
H	-3.44974600	-3.29040700	5.03709200
C	-4.00622900	-1.66371200	3.73683400
H	-4.51653300	-2.30235900	3.02006200
F	0.00548500	3.22586700	1.75377800

6. References

1. Cruz, C. A., Emslie, D. J. H., Harrington, L. E., Britten, J. F. & Robertson, C. M. Extremely Stable Thorium(IV) Dialkyl Complexes Supported by Rigid Tridentate 4,5-Bis(anilido)xanthene and 2,6-Bis(anilidomethyl)pyridine Ligands. *Organometallics* **26**, 692–701 (2007).
2. Han, X.-W., Daugulis, O. & Brookhart, M. Unsaturated Alcohols as Chain-Transfer Agents in Olefin Polymerization: Synthesis of Aldehyde End-Capped Oligomers and Polymers. *J. Am. Chem. Soc.* **142**, 15431–15437 (2020).
3. Itagaki, Y. *et al.* An ESR study on structures of a series of silylnitrenes. *Chem. Phys. Lett.* **348**, 249–254 (2001).
4. Wiberg, N. & Neruda, B. Silylazide, V. Darstellung, Eigenschaften und Struktur einiger Silylazide. *Chem. Ber.* **99**, 740–749 (1966).
5. Guschlbauer, J., Vollgraff, T., Xie, X., Fetoh, A. & Sundermeyer, J. Heavy silylchalcogenido lanthanates synthesis Ph4P[Cp3La–ESiMe3] (E = S, Se, and Te) via fluoride-induced demethylation of dimethylcarbonate to Ph4P[OCO2Me] key intermediate. *Dalton Trans.* **50**, 13103–13111 (2021).
6. Bejot, R., He, A., Falck, J. R. & Mioskowski, C. Chromium–Carbyne Complexes: Intermediates for Organic Synthesis. *Angew. Chem. Int. Ed.* **46**, 1719–1722 (2007).
7. Qi, X., Chen, P. & Liu, G. Catalytic Oxidative Trifluoromethoxylation of Allylic C−H Bonds Using a Palladium Catalyst. *Angew. Chem. Int. Ed.* **56**, 9517–9521 (2017).
8. McMullen, J. S., Edwards, A. J. & Hicks, J. C–H and C–F coordination of arenes in neutral alkaline earth metal complexes. *Dalton Trans.* **50**, 8685–8689 (2021).
9. Williams, D. E. Crystal Packing of Molecules. *Science* **147**, 605–606 (1965).
10. McCleverty, J. A., Locke, J., Wharton, E. J. & Gerloch, M. Transition-metal dithiolene complexes. Part IV. Trisdicyano-1,2-dithiolene complexes of first-row metals, and of molybdenum and tungsten. *J. Chem. Soc. Inorg. Phys. Theor.* 816–823 (1968) doi:10.1039/J19680000816.
11. Kläring, P., Jungton, A.-K., Braun, T. & Müller, C. Synthesis, Structure and Reactivity of Iridium Hydrido Fluorido Complexes. *Eur. J. Inorg. Chem.* **2012**, 1430–1436 (2012).
12. Bornemann, D. *et al.* Deoxygenative Fluorination of Phosphine Oxides: A General Route to Fluorinated Organophosphorus(V) Compounds and Beyond. *Angew. Chem. Int. Ed.* **59**, 22790–22795 (2020).
13. Scattolin, T., Deckers, K. & Schoenebeck, F. Direct Synthesis of Acyl Fluorides from Carboxylic Acids with the Bench-Stable Solid Reagent (Me4N)SCF3. *Org. Lett.* **19**, 5740–5743 (2017).
14. Bamford, K. L., Chitnis, S. S., Qu, Z. & Stephan, D. W. Interactions of C−F Bonds with Hydridoboranes: Reduction, Borylation and Friedel–Crafts Alkylation. *Chem. – Eur. J.* **24**, 16014–16018 (2018).
15. Wang, L. & Cornella, J. A Unified Strategy for Arylsulfur(VI) Fluorides from Aryl Halides: Access to Ar-SOF3 Compounds. *Angew. Chem. Int. Ed.* **59**, 23510–23515 (2020).
16. Zhang, X.-Y. *et al.* Reductive Catalytic Difluorocarbene Transfer via Palladium Catalysis. *Angew. Chem. Int. Ed.* **62**, e202306501 (2023).
17. Ortalli, S., Ford, J., Trabanco, A. A., Tredwell, M. & Gouverneur, V. Photoredox Nucleophilic (Radio)fluorination of Alkoxyamines. *J. Am. Chem. Soc.* **146**, 11599–11604 (2024).

18. Simmons, E. M. & Hartwig, J. F. On the Interpretation of Deuterium Kinetic Isotope Effects in C□H Bond Functionalizations by Transition-Metal Complexes. *Angew. Chem. Int. Ed.* **51**, 3066–3072 (2012).
19. Neese, F. Software Update: The ORCA Program System—Version 6.0. *WIREs Comput. Mol. Sci.* **15**, e70019 (2025).
20. Neese, F. The ORCA program system. *WIREs Comput. Mol. Sci.* **2**, 73–78 (2012).
21. Meng, E. C. *et al.* UCSF ChimeraX: Tools for structure building and analysis. *Protein Sci.* **32**, e4792 (2023).
22. Pettersen, E. F. *et al.* UCSF ChimeraX: Structure visualization for researchers, educators, and developers. *Protein Sci.* **30**, 70–82 (2021).
23. Grimme, S., Hansen, A., Ehlert, S. & Mewes, J.-M. r2SCAN-3c: A "Swiss army knife" composite electronic-structure method. *J. Chem. Phys.* **154**, 064103 (2021).
24. Furness, J. W., Kaplan, A. D., Ning, J., Perdew, J. P. & Sun, J. Accurate and Numerically Efficient r2SCAN Meta-Generalized Gradient Approximation. *J. Phys. Chem. Lett.* **11**, 8208–8215 (2020).
25. Brandenburg, J. G. *et al.* Geometrical Correction for the Inter- and Intramolecular Basis Set Superposition Error in Periodic Density Functional Theory Calculations. *J. Phys. Chem. A* **117**, 9282–9292 (2013).
26. Kruse, H. & Grimme, S. A geometrical correction for the inter- and intra-molecular basis set superposition error in Hartree-Fock and density functional theory calculations for large systems. *J. Chem. Phys.* **136**, 154101 (2012).
27. Neese, F. An improvement of the resolution of the identity approximation for the formation of the Coulomb matrix. *J. Comput. Chem.* **24**, 1740–1747 (2003).
28. Barone, V. & Cossi, M. Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model. *J. Phys. Chem. A* **102**, 1995–2001 (1998).
29. Garcia-Ratés, M. & Neese, F. Efficient implementation of the analytical second derivatives of hartree–fock and hybrid DFT energies within the framework of the conductor-like polarizable continuum model. *J. Comput. Chem.* **40**, 1816–1828 (2019).
30. Garcia-Ratés, M. & Neese, F. Effect of the Solute Cavity on the Solvation Energy and its Derivatives within the Framework of the Gaussian Charge Scheme. *J. Comput. Chem.* **41**, 922–939 (2020).
31. Chai, J.-D. & Head-Gordon, M. Long-range corrected hybrid density functionals with damped atom–atom dispersion corrections. *Phys. Chem. Chem. Phys.* **10**, 6615–6620 (2008).
32. Müller, M., Hansen, A. & Grimme, S. ωB97X-3c: A composite range-separated hybrid DFT method with a molecule-optimized polarized valence double-ζ basis set. *J. Chem. Phys.* **158**, 014103 (2023).
33. Weigend, F. & Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **7**, 3297–3305 (2005).
34. Helmich-Paris, B., de Souza, B., Neese, F. & Izsák, R. An improved chain of spheres for exchange algorithm. *J. Chem. Phys.* **155**, 104109 (2021).
35. Weigend, F. Accurate Coulomb-fitting basis sets for H to Rn. *Phys. Chem. Chem. Phys.* **8**, 1057–1065 (2006).
36. Neese, F., Hansen, A. & Liakos, D. G. Efficient and accurate approximations to the local coupled cluster singles doubles method using a truncated pair natural orbital basis. *J. Chem. Phys.* **131**, 064103 (2009).

37. Neese, F., Wennmohs, F. & Hansen, A. Efficient and accurate local approximations to coupled-electron pair approaches: An attempt to revive the pair natural orbital method. *J. Chem. Phys.* **130**, 114108 (2009).
38. Riplinger, C. & Neese, F. An efficient and near linear scaling pair natural orbital based local coupled cluster method. *J. Chem. Phys.* **138**, 034106 (2013).
39. Riplinger, C., Sandhoefer, B., Hansen, A. & Neese, F. Natural triple excitations in local coupled cluster calculations with pair natural orbitals. *J. Chem. Phys.* **139**, 134101 (2013).
40. Riplinger, C., Pinski, P., Becker, U., Valeev, E. F. & Neese, F. Sparse maps—A systematic infrastructure for reduced-scaling electronic structure methods. II. Linear scaling domain based pair natural orbital coupled cluster theory. *J. Chem. Phys.* **144**, 024109 (2016).
41. Schneider, W. B. *et al.* Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework. *J. Chem. Theory Comput.* **12**, 4778–4792 (2016).
42. Bistoni, G. *et al.* Treating Subvalence Correlation Effects in Domain Based Pair Natural Orbital Coupled Cluster Calculations: An Out-of-the-Box Approach. *J. Chem. Theory Comput.* **13**, 3220–3227 (2017).
43. Hellweg, A., Hättig, C., Höfener, S. & Klopper, W. Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. *Theor. Chem. Acc.* **117**, 587–597 (2007).
44. Wuttke, A. & Mata, R. A. Visualizing dispersion interactions through the use of local orbital spaces. *J. Comput. Chem.* **38**, 15–23 (2017).
45. Altun, A., Neese, F. & Bistoni, G. Effect of Electron Correlation on Intermolecular Interactions: A Pair Natural Orbitals Coupled Cluster Based Local Energy Decomposition Study. *J. Chem. Theory Comput.* **15**, 215–228 (2019).
46. Mitoraj, M. P., Michalak, A. & Ziegler, T. A Combined Charge and Energy Decomposition Scheme for Bond Analysis. *J. Chem. Theory Comput.* **5**, 962–975 (2009).
47. Lu, T. A comprehensive electron wavefunction analysis toolbox for chemists, Multiwfn. *J. Chem. Phys.* **161**, 082503 (2024).
48. Lu, T. & Chen, F. Multiwfn: A multifunctional wavefunction analyzer. *J. Comput. Chem.* **33**, 580–592 (2011).
49. Todd A. Keith. AIMALL. TK Gristmill Software (2019).
50. E. D. Glendening *et al.* NBO 7.0. Theoretical Chemistry Institute, University of Wisconsin (2018).
51. Glendening, E. D., Landis, C. R. & Weinhold, F. NBO 7.0: New vistas in localized and delocalized chemical bonding theory. *J. Comput. Chem.* **40**, 2234–2241 (2019).