The Perfluoroadamantoxy Aluminate as an Ideal Weakly Coordinating Anion? - Synthesis and first Applications.

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Content

General Considerations

All manipulations were carried out in an inert gas atmosphere of argon, using standard vacuum and Schlenk techniques with a vacuum of 10^{-3} mbar or a glove box (MBraun Lab Master) with argon atmosphere and H_2O and O_2 contents <1 ppm to exclude air and moisture. All glassware used in reactions have been stored in a drying oven at 180 °C overnight and were additionally dried with a heat gun prior to use. Unless stated otherwise all reactions were performed in special double-Schlenk tubes separated by a G3 or G4 frit and equipped with grease-free PTFE or glass valves. All solvents and reagents were dried using conventional drying agents, distilled afterwards and stored under argon atmosphere over activated 3 Å molecular sieves.

NMR Spectroscopy

NMR samples were prepared in an inert atmosphere glove box in NMR tubes equipped with a gas-tight J. Young valve. NMR spectra were recorded on a Bruker Avance II$^+$ 400 MHz WB, Bruker Avance III HD 300 MHz and a Bruker Avance DPX 200 MHz NMR spectrometer at room temperature (unless described otherwise) using the software package Bruker TopSpin 4.0.7 for analysis. The spectra were calibrated based on the chemical shift of the solvents used. Since most measured spectra did not contain deuterated solvents, *o*-DFB and THF were first measured with CD_2Cl_2 alone to obtain uniform calibration values. The obtained calibration values for the ^{1}H-NMR spectra are shown in the following table:

Data for NMR calibration.

solvents	Chemical shift: δ(^{1}H) [ppm]
CD_3CN	1.96[1]
$CDCl_3$	7.26[1]
CD_2Cl_2	5.33[1]
o-DFB	7.19[a]
THF	1.79[b][1]
	3.62[c][1]

[a] = centre of the m, [b] = (CH_2 (3,4)), [c] = (CH_2 (2,5))

The field correction of the heteronuclear NMR spectra were referenced to LiCl in D_2O for the ^{7}Li spectra, to $BF_3{\cdot}Et_2O$ for the ^{11}B spectra, to Me_4Si for the ^{13}C spectra, to $CFCl_3$ for the ^{19}F spectra, to NaCl in D_2O for the ^{23}Na spectra, to a 1.1 M solution of $Al(NO_3)_3$ in D_2O for the ^{27}Al spectra and 85 % H_3PO_4 for the ^{31}P NMR spectra.[2]

Vibrational Spectroscopy

Raman spectroscopy was performed at r.t. with a Bruker VERTEX 70 spectrometer equipped with a Bruker RAM II module (Nd/YAG 1064 nm laser) with a nitrogen cooled Ge detector. The samples were measured in sealed soda-lime glass Pasteur pipettes or in NMR tubes equipped with a gas-tight J. Young valve in the region of 4000 to 200 cm^{-1} with a resolution of 4 cm^{-1} with 1000 scans.

ATR FTIR spectroscopy was performed at r.t. with a diamond crystal on a Bruker ALPHA spectrometer with a QuickSnap Platinum ATR sampling module inside an inert atmosphere glovebox. A KBr beam splitter was used for the spectral range from 4000 to 400 cm^{-1}. The spectra were recorded with 64 scans and resolution of 2 cm^{-1}. Data processing was carried out with the software package OPUS 7.5 and OriginPro 2019b. Unless stated different, the usual processing procedure included a baseline

correction with one iteration and a standardization of the signal intensities. The relative band intensities were described as follows: ≥ 0.8 = very strong (vs), ≥ 0.6 = strong (s), ≥ 0.4 = medium (m), ≥ 0.2 = weak (w), < 0.2 = very weak (vw).

Single Crystal X-ray Diffration

Single-crystal X-ray data were collected on a Bruker SMART APEXII QUAZAR three-circle diffractometer with a microfocus sealed X-ray tube using Incoatec mirror optics as a monochromator. Mo-K_α radiation (λ = 0.71073 Å) was used for all measurements. The obtained crystals were coated with perfluoropolyalkylether oil (AB128330, ABCR GmbH & Co. KG), mounted on 0.1 to 0.3 mm micromounts and shock-cooled to 100 K on the diffractometer (using an Oxford Cryosystem open flow N_2 cooling device).[3] All data were integrated with SAINT[4], a multi-scan absorption-correction using SADABS-2016/2 was applied.[5]The structures were solved by direct methods using SHELXT 2014/5[6] and refined by full-matrix least-squares methods against F^2 by SHELXL-2018/3[7] employing the shelXle GUI (Revision 1449).[8] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond-length restraints and displacement-parameter restraints. Some parts of the disorder model were introduced by the program DSR.[9,10] The cif files were generated using FinalCif.[10,11] Graphical representations were prepared using the software OLEX2 (version 1.3.0).[12]

Computational Details

Unless stated otherwise, quantum chemical calculations were carried out with the TURBOMOLE software[13] (v7.2 or v7.5) in the highest possible point group using the DFT functional BP86[14] (the resolution-of-identity RI approximation[15]) in combination with the def-SV(P)[16] and def-TZVPP[17] basis sets and D3 dispersion correction with Becke-Johnson (BJ) damping[18], a fine integration grid (m3 or m4) and the default SCF convergence criteria (10^{-6} a.u.). Every species presented herein was checked in terms of reasonable geometry and electronic occupation with the EIGER module. Vibrational frequencies were calculated analytically using the AOFORCE module.[19] All structures represented true minima without imaginary frequencies on the respective hypersurface. Thermodynamic terms were calculated with inclusion of zero-point energy and thermal contributions to the enthalpy/entropy (FREEH tool; unscaled BP86 vibrational frequencies). Gibbs free energies of solvation were calculated with the COSMO model.[20] Detailed descriptions of the performed calculations are given prior to the obtained data for each chapter.

Experimental Details

Characterization of $C_{10}F_{15}OH$

^{1}H-NMR (200.13 MHz, 298 K, CD_2Cl_2): δ = 4.01 (br. s, 1H, $C_{10}F_{15}$O**H**) ppm.
^{19}F-NMR (188.31 MHz, 298 K, CD_2Cl_2): δ = −222.4 (m, C**F**, 3F, $C_{10}F_{15}OH$), −121.1 (m, C**F_2**, 12F, $C_{10}F_{15}OH$) ppm.
FTIR (Diamant, ATR): $\tilde{\nu}$ = 3594 (vw), 3573 (vw), around 3470 (very broad, vw), 1364 (vw), 1299 (vw), 1263 (vs), 1256 (vs), 1210 (vw), 1159 (vw), 1095 (vw), 1055 (vw), 992 (vw), 958 (s), 940 (vs), 842 (vw), 650 (s), 571 (vw), 461 (vw), 441 (s), 410 (vw), 402 (vw) cm^{-1}.
FT-Raman: $\tilde{\nu}$ = 1294 (m), 1062 (vw), 701 (w), 574 (s), 443 (w), 371 (vs), 313 (vs), 264 (vw) cm^{-1}.

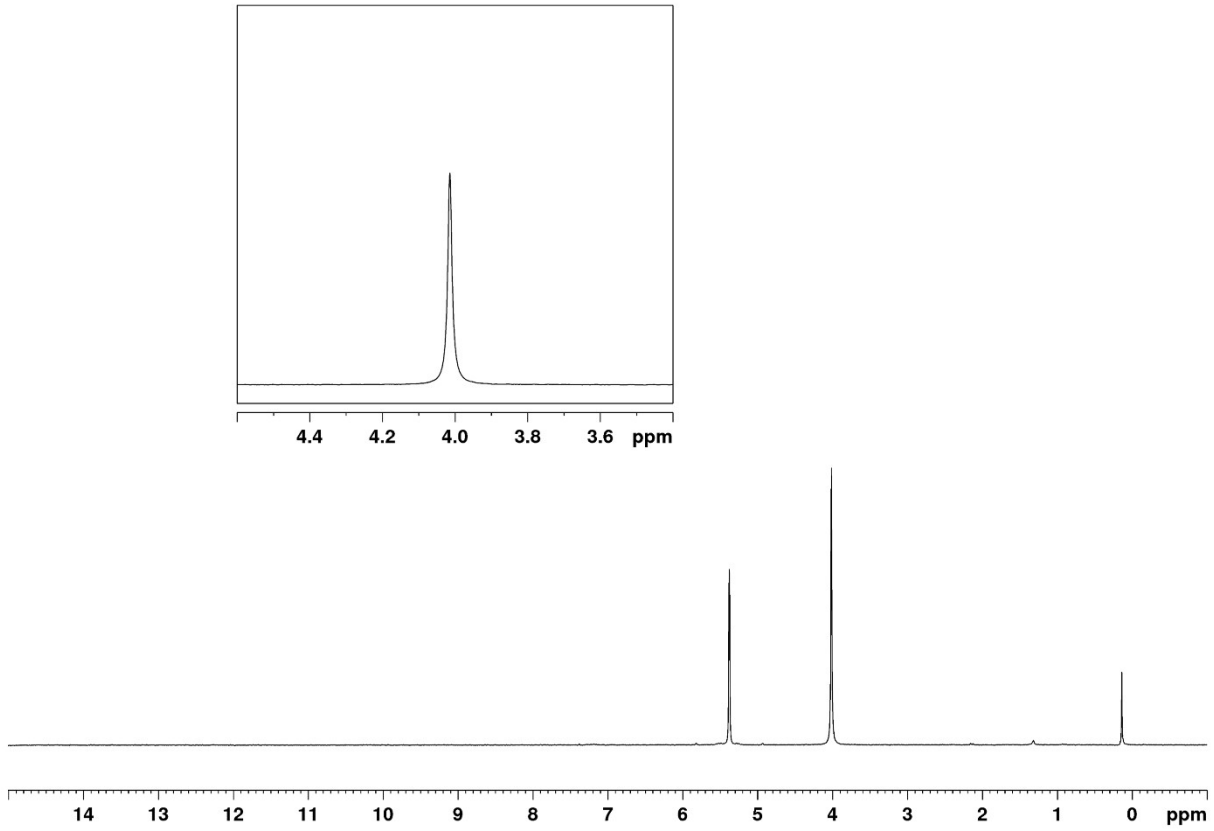


Figure S- 1: ^{1}H-NMR spectrum (200.13 MHz, 298 K, CD_2Cl_2) of dried $C_{10}F_{15}OH$.

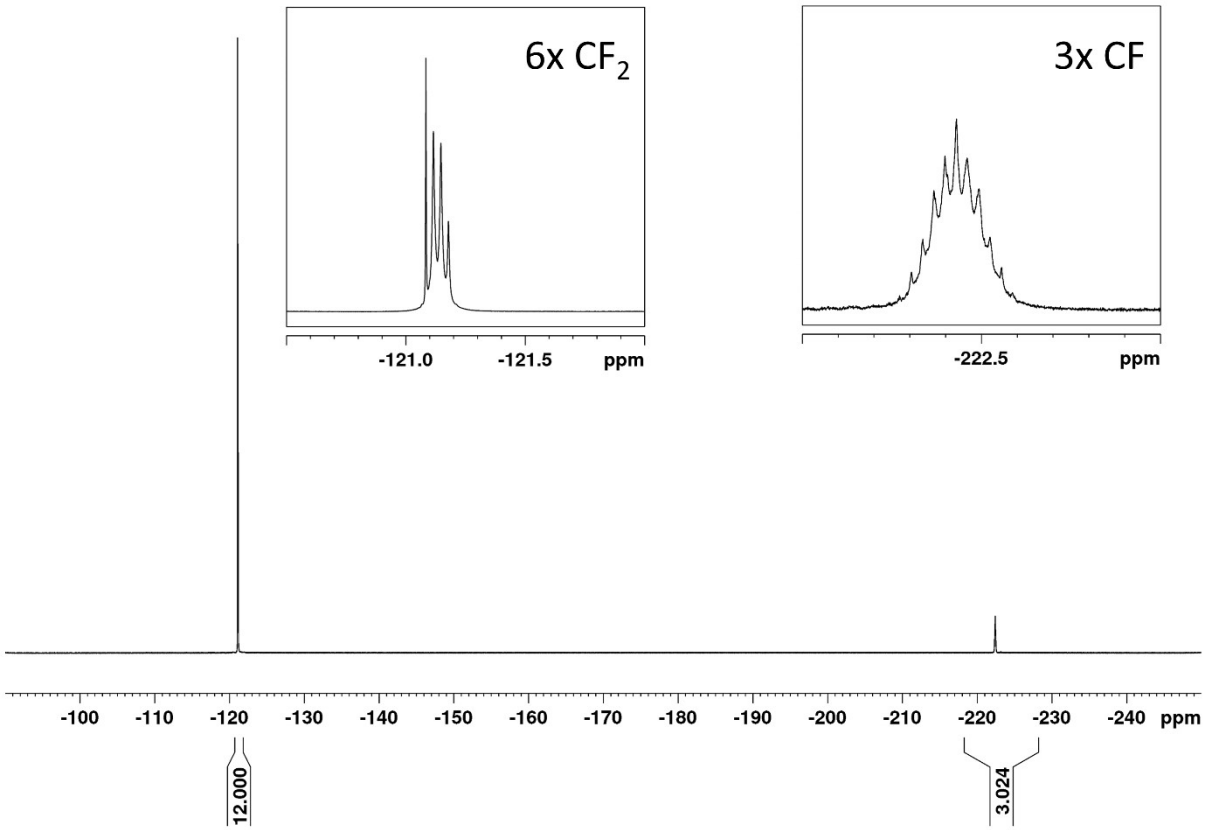


Figure S- 2: ^{19}F-NMR spectrum (188.31 MHz, 298 K, CD_2Cl_2) of dried $C_{10}F_{15}OH$.

Synthesis of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurities of C$_{10}$F$_{15}$OH

Purified and slightly ground $LiAlH_4$ (20.2 mg, 0.532 mmol) and perfluoro-1-adamantanol (1.04 g, 2.46 mmol, 4.62 eq) (**Note:** Since $C_{10}F_{15}OH$ can be sublimed at 50°C in dynamic vacuo, it was used in large excess and reclaimed during working up) were submitted into a Schlenk flask and suspended in *o*-DFB (40 mL). The reaction mixture was stirred for 2 h 10 min under reflux until the evolution of gas was finished. The solvent was removed under reduced pressure and the obtained colorless solid (0.85 g, 0.50 mmol, 94 %) was analyzed by NMR spectroscopy showing impurity of unreacted alcohol $C_{10}F_{15}OH$ ($Li[Al(OC_{10}F_{15})_4]$: $C_{10}F_{15}OH$ = 0.39 : 1.0 by integration of the CF groups).

^{1}H-NMR (300.18 MHz, 298 K, CD_2Cl_2/*o*-DFB): δ = 4.10 (br. s, 1H, $C_{10}F_{15}O$**H**) ppm.
^{7}Li-NMR (116.66 MHz, 298 K, CD_2Cl_2/*o*-DFB): δ = −0.1 (s, 1Li, **Li**[Al(OC$_{10}$F$_{15}$)$_4$]) ppm.
^{19}F-NMR (282.45 MHz, 298 K, CD_2Cl_2/*o*-DFB): δ = −223.2 (m, C**F**, 12F, Li[Al(OC$_{10}$F$_{15}$)$_4$]), −222.6 (m, C**F**, 3F, $C_{10}F_{15}OH$), −121.4 (m, C**F$_2$**, 48F, Li[Al(OC$_{10}$F$_{15}$)$_4$]), −121.3 (chemical shift not exactly determinable due to overlapping, C**F$_2$**, 12F, $C_{10}F_{15}OH$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, CD_2Cl_2/*o*-DFB): δ = 35.2 (s, 1Al, Li[**Al**(OC$_{10}$F$_{15}$)$_4$]) ppm.

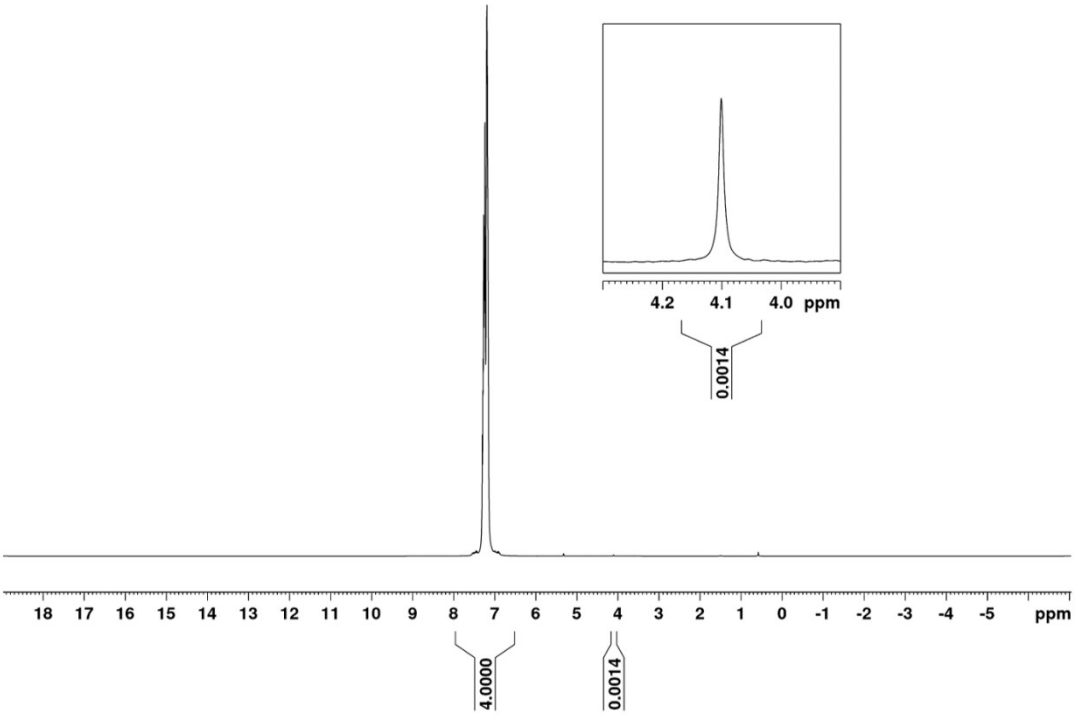


Figure S- 3: ^{1}H-NMR spectrum (300.18 MHz, 298 K, CD_2Cl_2/*o*-DFB) of $Li[Al(OC_{10}F_{15})_4]$ containing impurity.

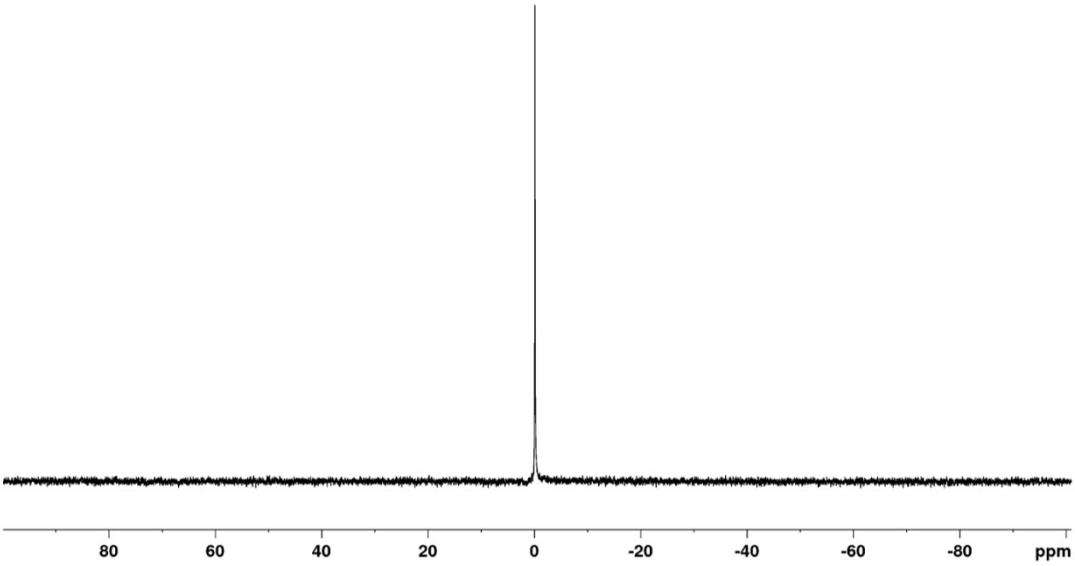


Figure S- 4: ^{7}Li-NMR spectrum (116.66 MHz, 298 K, CD_2Cl_2/*o*-DFB) of $Li[Al(OC_{10}F_{15})_4]$ containing impurity.

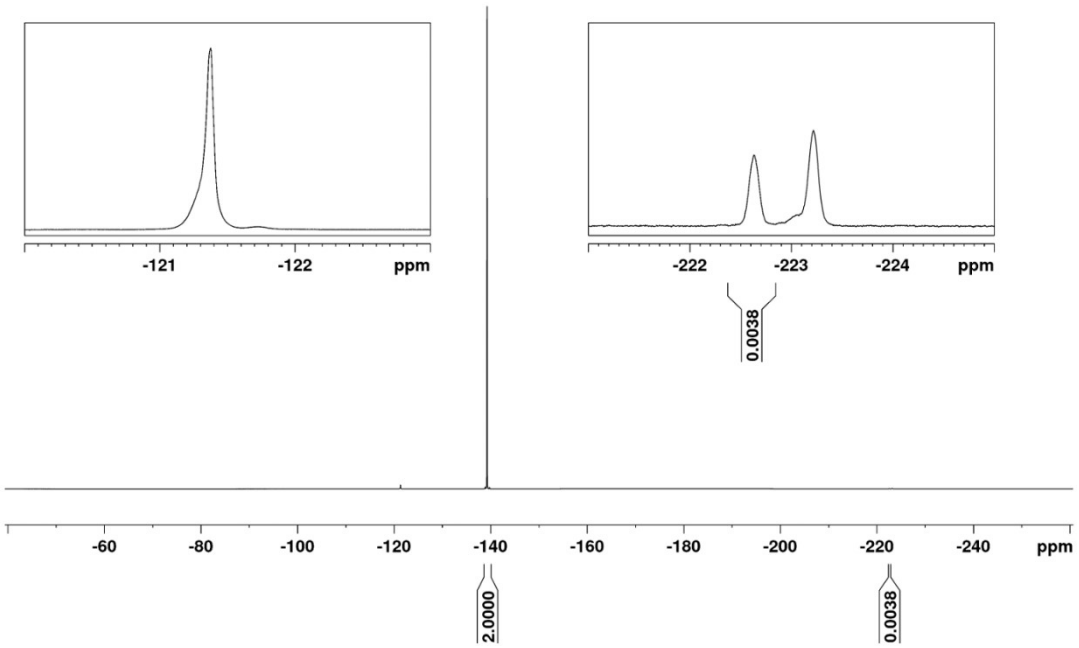


Figure S- 5: ^{19}F-NMR spectrum (282.45 MHz, 298 K, CD_2Cl_2/*o*-DFB) of $Li[Al(OC_{10}F_{15})_4]$ containing impurity.

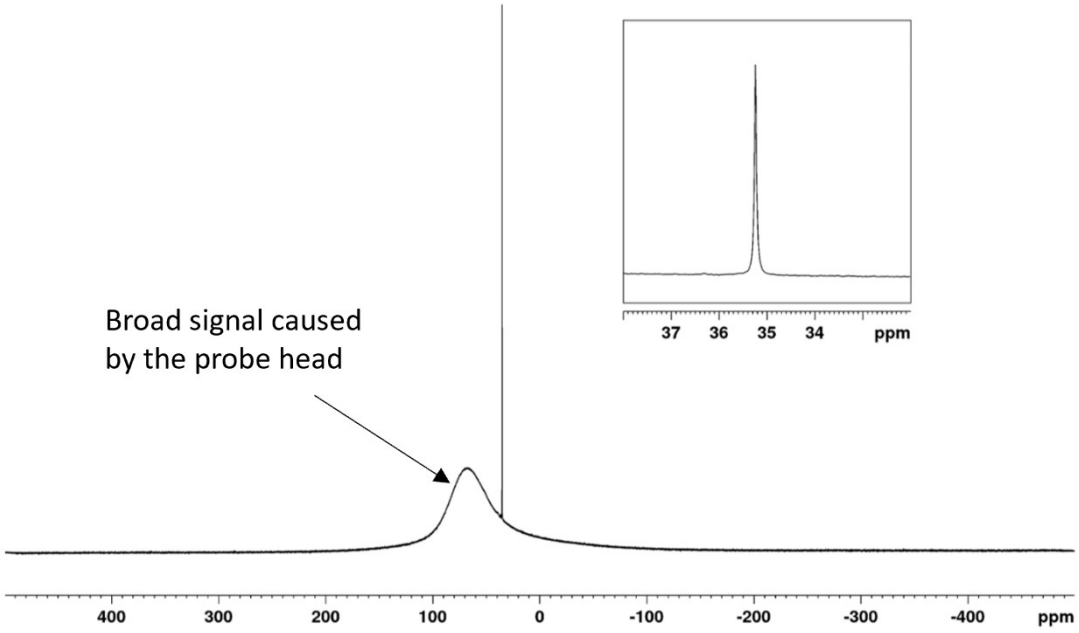


Figure S- 6: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, CD_2Cl_2/*o*-DFB) of $Li[Al(OC_{10}F_{15})_4]$ containing impurity.

This attempt was washed with toluene (2x 15 mL) (**Note:** The target compound $Li[Al(OC_{10}F_{15})_4]$ is insoluble in toluene in contrast to $C_{10}F_{15}OH$), dried in dynamic vacuo and analyzed via NMR spectroscopy twice, before and after addition of a small amount of further alcohol $C_{10}F_{15}OH$ to identify the impurity as unreacted alcohol.

Black: Before addition of $C_{10}F_{15}OH$. Blue: After addition of $C_{10}F_{15}OH$. Red: Difference

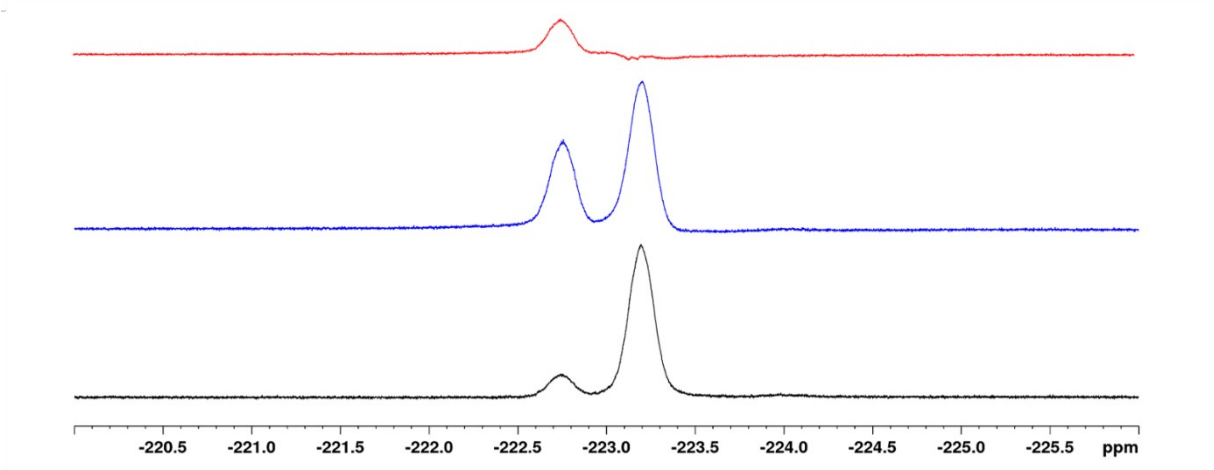


Figure S- 7: ^{19}F-NMR spectrum (188.31 MHz, 298 K, *o*-DFB) Comparison of the resonances at –222.8 ppm before (black), after addition of further $C_{10}F_{15}OH$ (blue) and difference spectrum of these two spectra (red).

Synthesis of $Li[Al(OC_{10}F_{15})_4]$ containing impurities of $C_{10}F_{15}OH$ after prolonged reaction time

Purified and slightly ground $LiAlH_4$ (71.0 mg, 1.87 mmol) and perfluoro-1-adamantanol (3.25 g, 7.70 mmol, 4.11 eq) were submitted into a Schlenk flask and suspended in *o*-DFB (20 mL). The reaction mixture was stirred for 3 days under reflux. The solvent was removed under reduced pressure and the obtained colorless solid (2.90 g, 0.500 mmol, 90.0 %) was analyzed by NMR spectroscopy showing impurity of unreacted alcohol $C_{10}F_{15}OH$ ($Li[Al(OC_{10}F_{15})_4]$: $C_{10}F_{15}OH$ = 1.0 : 0.4 by integration of the CF groups) (**Note:** The obvious chemical shift downfield in the ^{1}H-NMR spectrum of $C_{10}F_{15}O$**H** is attributed to the use of THF as solvent).

^{1}H-NMR (300.18 MHz, 298 K, THF): δ = 9.58 (br. s, 1H, $C_{10}F_{15}O$**H**) ppm.
^{7}Li-NMR (116.66 MHz, 298 K, THF): δ = −0.5 (s, 1Li, **Li**$[Al(OC_{10}F_{15})_4]$) ppm.
^{19}F-NMR (282.45 MHz, 298 K, THF): δ = −224.0 (m, C**F**, 12F, $Li[Al(OC_{10}F_{15})_4]$), −223.5 (m, C**F**, 3F, $C_{10}F_{15}OH$), −140.1 (m, C**F**, 2F, *o*-DFB), −122.0 (m, C**F$_2$**, 48F, $Li[Al(OC_{10}F_{15})_4]$), −121.8 (chemical shift not exactly determinable due to overlapping, C**F$_2$**, 12F, $C_{10}F_{15}OH$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, THF): δ = 34.6 (s, 1Al, $Li[$**Al**$(OC_{10}F_{15})_4]$) ppm.

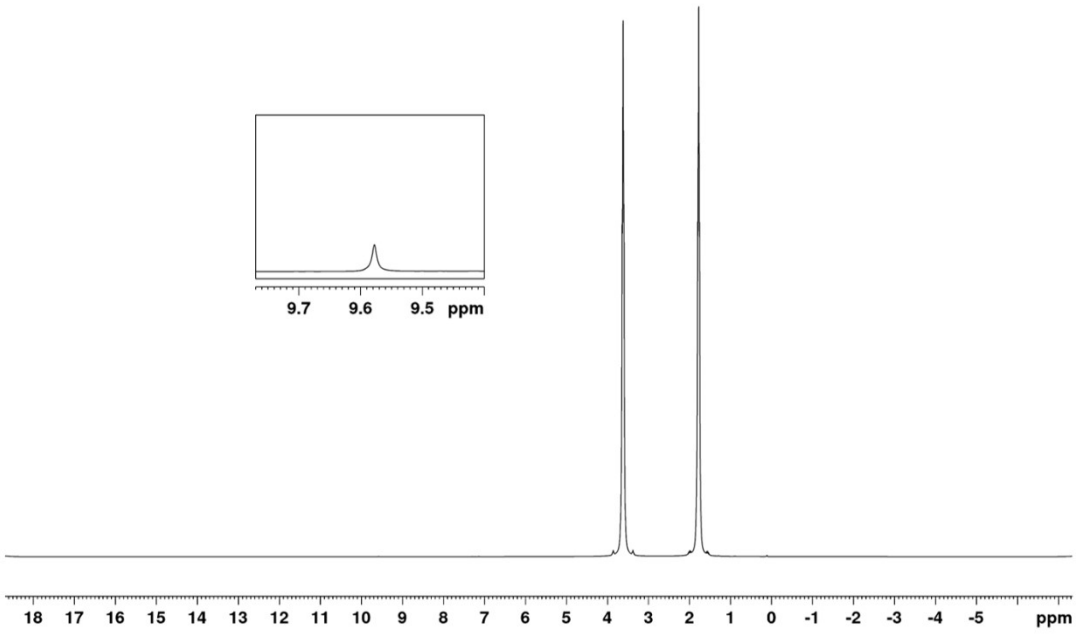


Figure S- 8: ^{1}H-NMR spectrum (300.18 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurity after 3 d of heating.

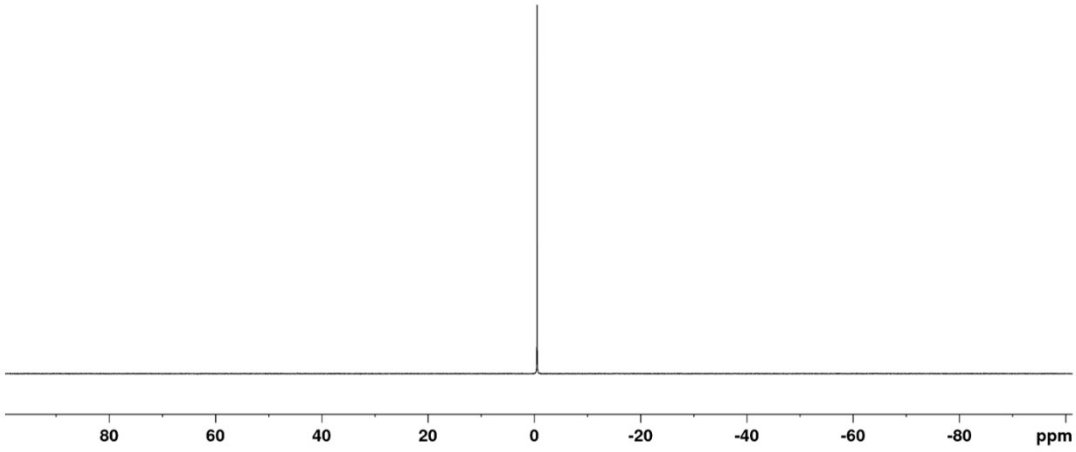


Figure S- 9: ^{7}Li-NMR spectrum (116.66 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurity after 3 d of heating.

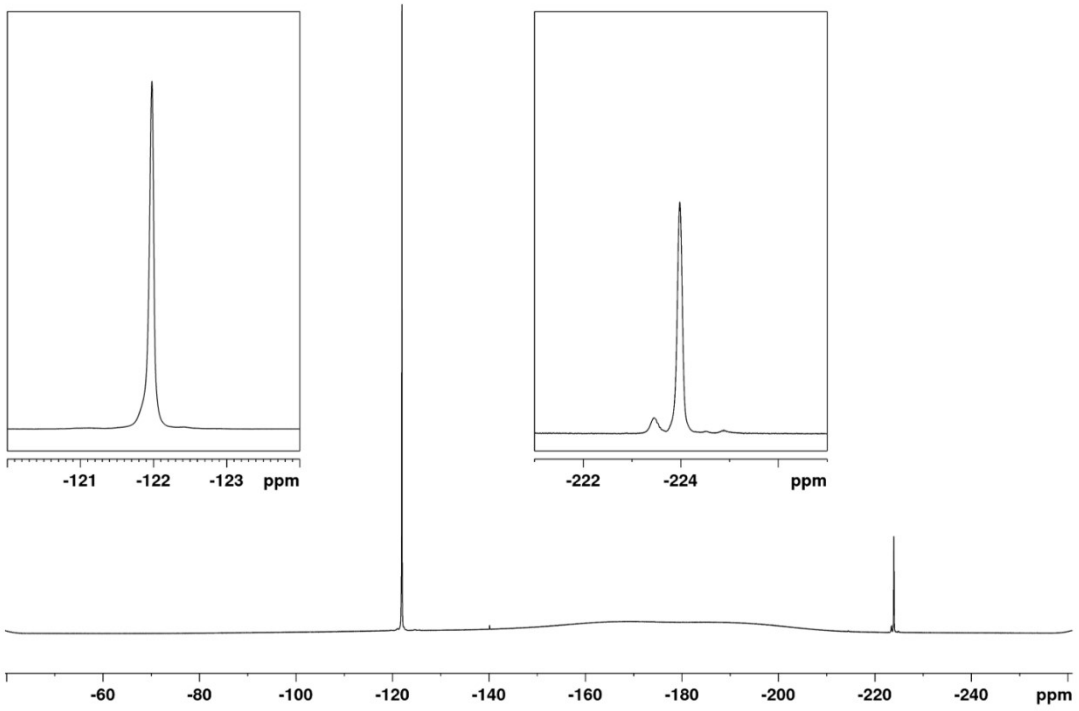


Figure S- 10: ^{19}F-NMR spectrum (282.45 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurity after 3 d of heating.

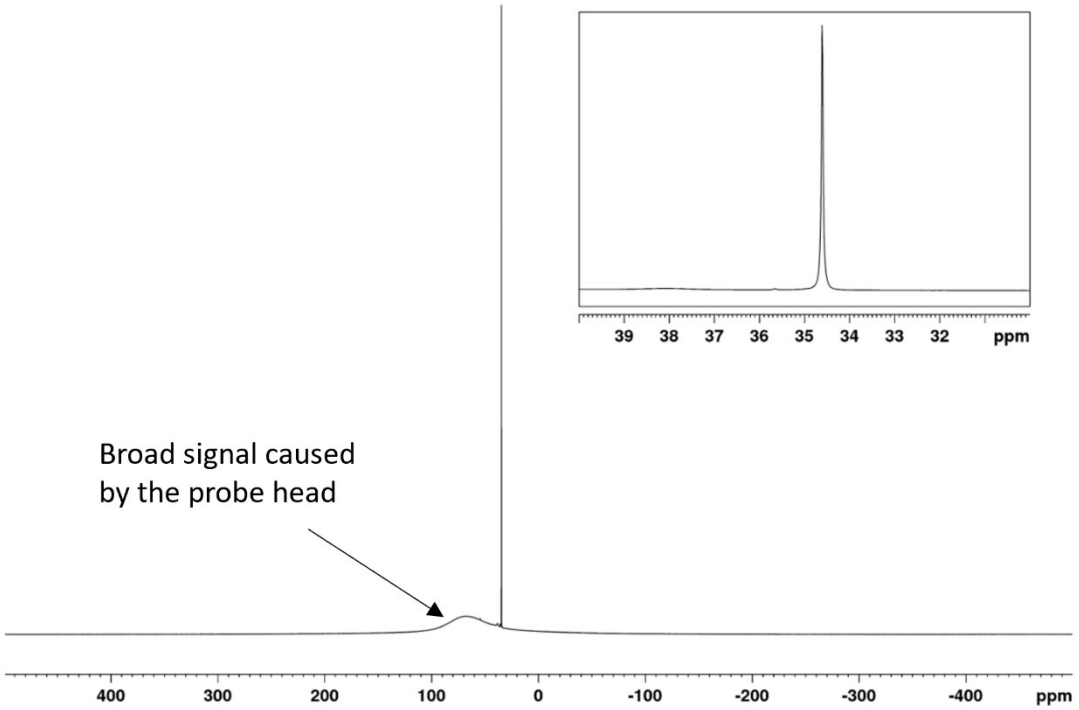


Figure S- 11: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurity after 3 d of heating.

Synthesis of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurities of C$_{10}$F$_{15}$OH after prolonged reaction time with less than 4.0 eq. of C$_{10}$F$_{15}$OH

Purified and slightly ground $LiAlH_4$ (7.6 mg, 0.20 mmol) and perfluoro-1-adamantanol (0.314 g, 0.744 mmol, 3.71 eq) were submitted into a Schlenk flask and suspended in *o*-DFB (5 mL). The reaction

mixture was stirred at room temperature overnight and afterwards stirred for 8 h under reflux. The solvent was removed under reduced pressure and the obtained colorless solid was washed with toluene (12.0 mL), dried under reduced pressure at slightly elevated temperature (0.271 g, 0.158 mmol, 78.8 %) and analyzed by NMR spectroscopy showing impurity of unreacted alcohol $C_{10}F_{15}OH$ ($Li[Al(OC_{10}F_{15})_4]$: $C_{10}F_{15}OH$ = 1.0 : 0.43 by integration of the CF groups) (**Note:** The obvious chemical shift downfield in the ^{1}H-NMR spectrum of $C_{10}F_{15}O$**H** is attributed to the use of THF as solvent).

^{1}H-NMR (300.18 MHz, 298 K, THF): δ = 9.58 (br. s, 1H, $C_{10}F_{15}O$**H**) ppm.
^{7}Li-NMR (116.66 MHz, 298 K, THF): δ = −0.5 (s, 1Li, **Li**$[Al(OC_{10}F_{15})_4]$) ppm.
^{19}F-NMR (282.45 MHz, 298 K, THF): δ = −224.0 (m, C**F**, 12F, $Li[Al(OC_{10}F_{15})_4]$), −223.5 (m, C**F**, 3F, $C_{10}F_{15}OH$), −140.1 (m, C**F**, 2F, *o*-DFB), −122.0 (m, C**F$_2$**, 48F, $Li[Al(OC_{10}F_{15})_4]$), −121.8 (chemical shift not exactly determinable due to overlapping, C**F$_2$**, 12F, $C_{10}F_{15}OH$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, THF): δ = 34.6 (s, 1Al, $Li[$**Al**$(OC_{10}F_{15})_4]$) ppm.

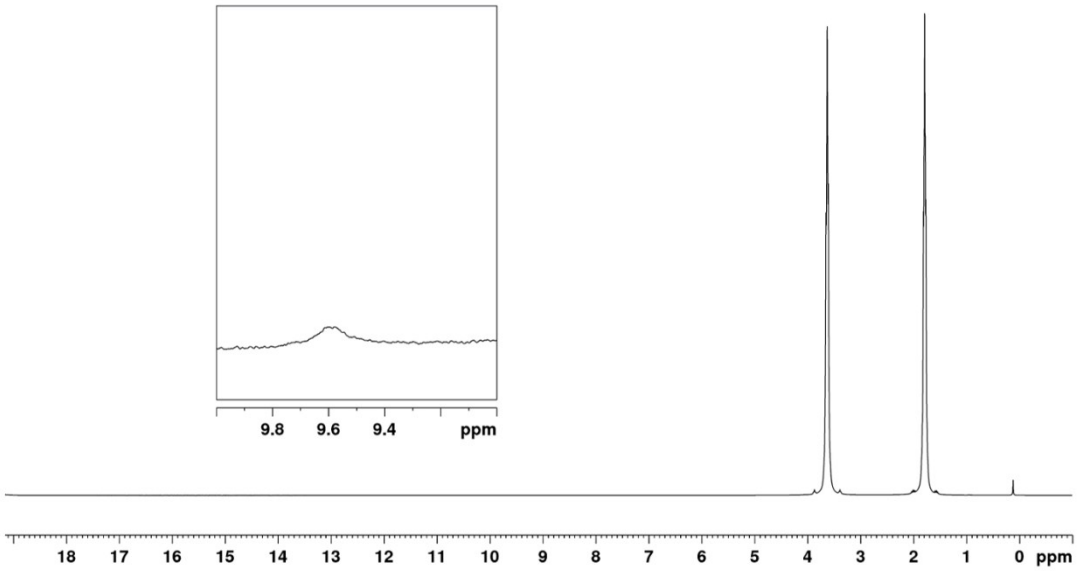


Figure S- 12: ^{1}H-NMR spectrum (300.18 MHz, 298 K, THF) of $Li[Al(OC_{10}F_{15})_4]$ containing impurities of $C_{10}F_{15}OH$ after prolonged reaction time with less than 4.0 eq. of $C_{10}F_{15}OH$.

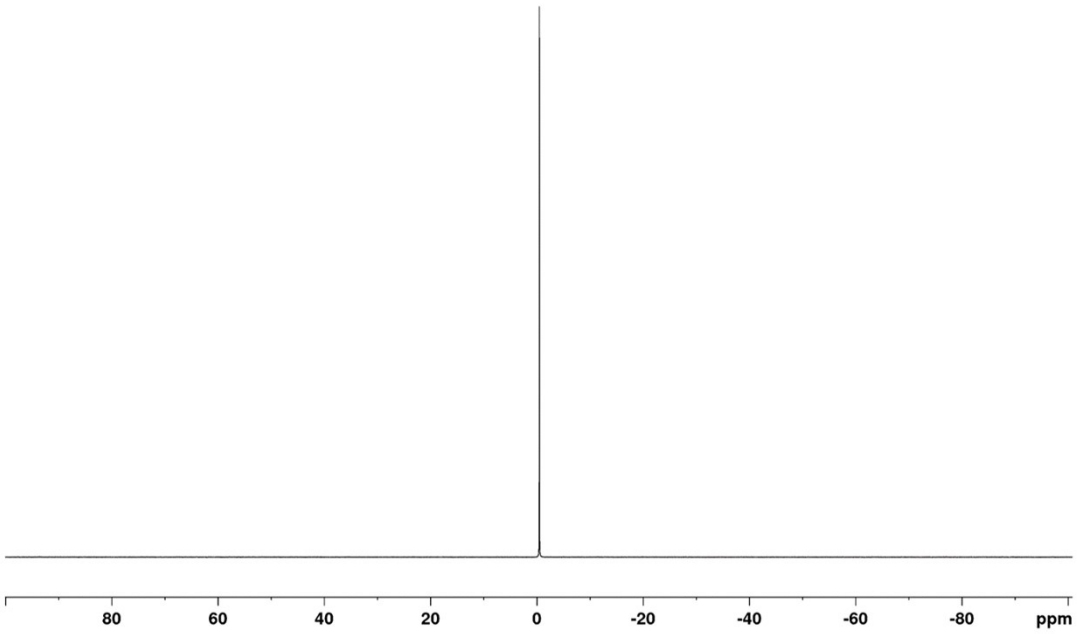


Figure S- 13: ^{7}Li-NMR spectrum (116.66 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurities of C$_{10}$F$_{15}$OH after prolonged reaction time with less than 4.0 eq. of C$_{10}$F$_{15}$OH.

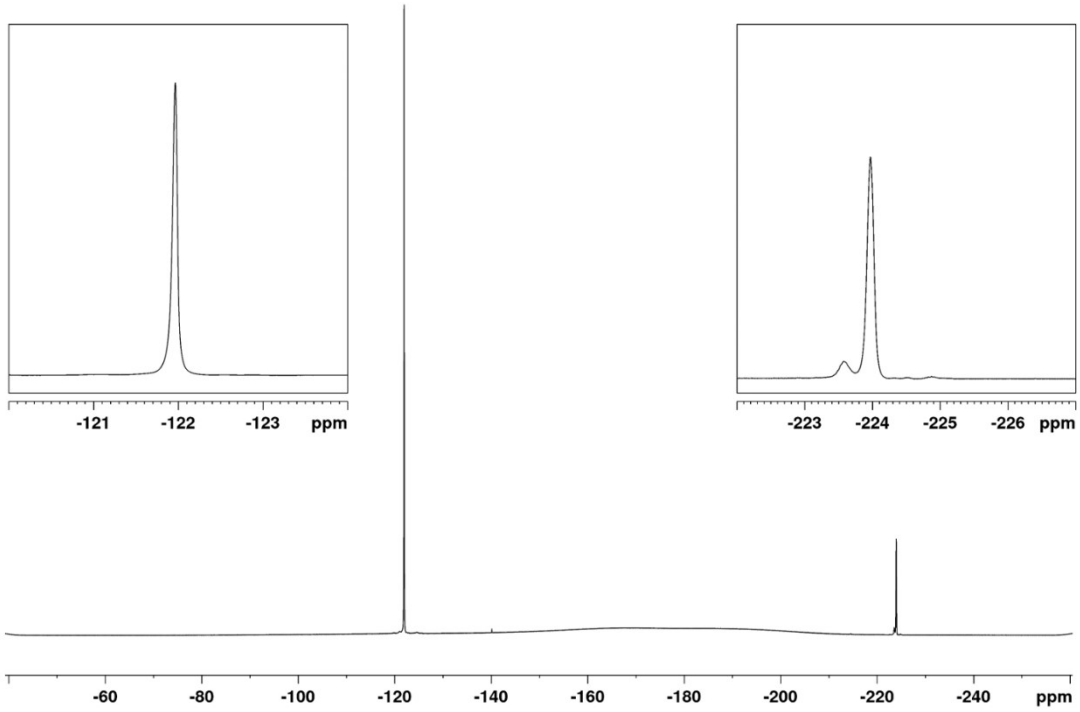


Figure S- 14: ^{19}F-NMR spectrum (282.45 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurities of C$_{10}$F$_{15}$OH after prolonged reaction time with less than 4.0 eq. of C$_{10}$F$_{15}$OH.

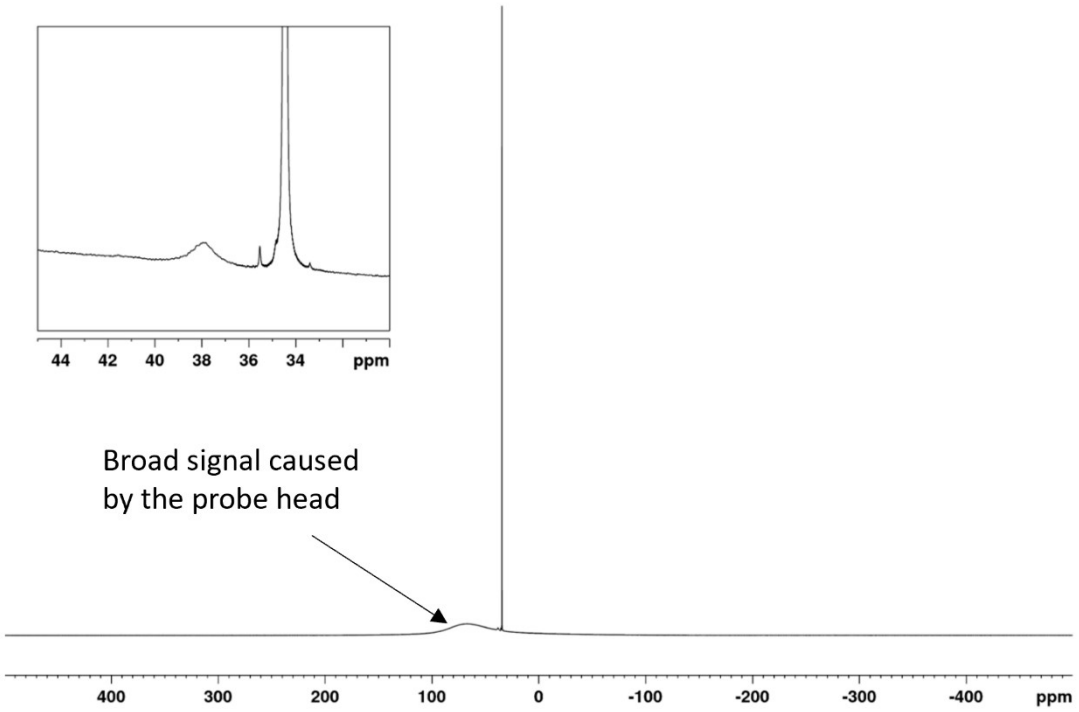


Figure S- 15: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurity of C$_{10}$F$_{15}$OH after prolonged reaction time with less than 4.0 eq. of C$_{10}$F$_{15}$OH.

Ideal synthesis protocol for Li[Al(OC$_{10}$F$_{15}$)$_4$]·(C$_{10}$F$_{15}$OH)$_x$

Purified and slightly ground $LiAlH_4$ (0.100 g, 2.64 mmol) and perfluoro-1-adamantanol (5.005 g, 11.86 mmol, 4.50 eq) were submitted into a Schlenk flask and suspended in *o*-DFB (40 mL). The reaction mixture was stirred for 3 h under reflux. The solvent was removed under reduced pressure, the obtained colorless solid was washed with toluene (3x, 20 mL), dried under reduced pressure at 100°C for 3 h (4.80 g, 2.53 mmol, 96 %) and analyzed by NMR spectroscopy showing impurity of unreacted alcohol C$_{10}$F$_{15}$OH (Li[Al(OC$_{10}$F$_{15}$)$_4$] : C$_{10}$F$_{15}$OH = 1.0 : 0.43 by integration of the CF groups) (**Note:** The obvious chemical shift downfield in the ^{1}H-NMR spectrum of C$_{10}$F$_{15}$O**H** is attributed to the use of THF as solvent; the yield was determined by use of the calculated molar mass of 1891.74 g·mol^{-1} for Li[Al(OC$_{10}$F$_{15}$)$_4$]·(C$_{10}$F$_{15}$OH)$_x$ with x = 0.43).

^{1}H-NMR (300.18 MHz, 298 K, THF): δ = 9.58 (br. s, 1H, C$_{10}$F$_{15}$O**H**) ppm.
^{7}Li-NMR (116.66 MHz, 298 K, THF): δ = −0.5 (s, 1Li, **Li**[Al(OC$_{10}$F$_{15}$)$_4$]) ppm.
^{19}F-NMR (282.45 MHz, 298 K, THF): δ = −224.0 (m, C**F**, 12F, Li[Al(OC$_{10}$F$_{15}$)$_4$]), −223.4 (m, C**F**, 3F, C$_{10}$F$_{15}$OH), −140.2 (m, C**F**, 2F, *o*-DFB), −122.0 (m, C**F$_2$**, 48F, Li[Al(OC$_{10}$F$_{15}$)$_4$]), −121.8 (chemical shift not exactly determinable due to overlapping, C**F$_2$**, 12F, C$_{10}$F$_{15}$OH) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, THF): δ = 34.6 (s, 1Al, Li[**Al**(OC$_{10}$F$_{15}$)$_4$]) ppm.

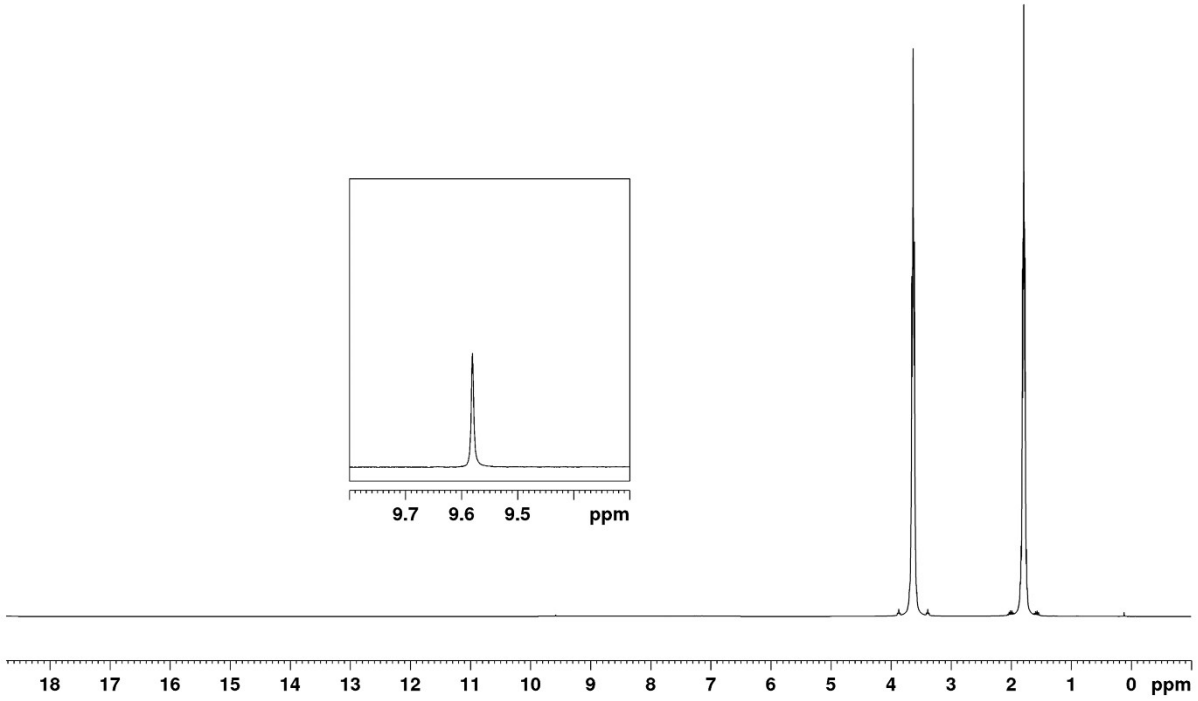


Figure S- 16: ^{1}H-NMR spectrum (300.18 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurity of 0.43 eq of C$_{10}$F$_{15}$OH.

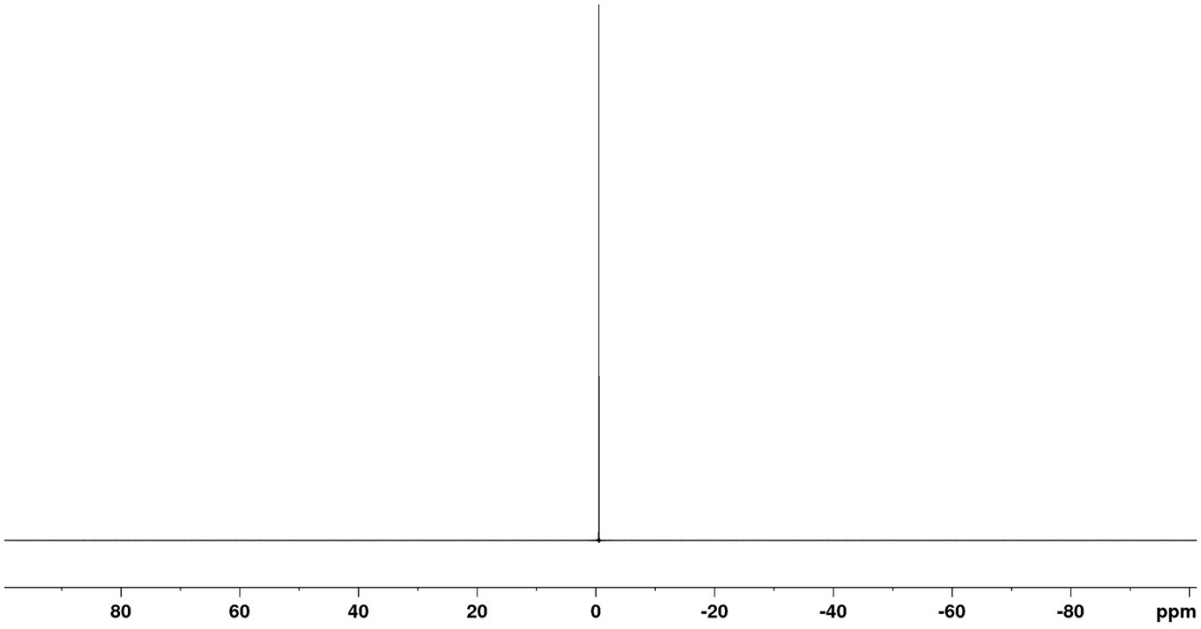


Figure S- 17: ^{7}Li-NMR spectrum (116.66 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurity of 0.43 eq of C$_{10}$F$_{15}$OH.

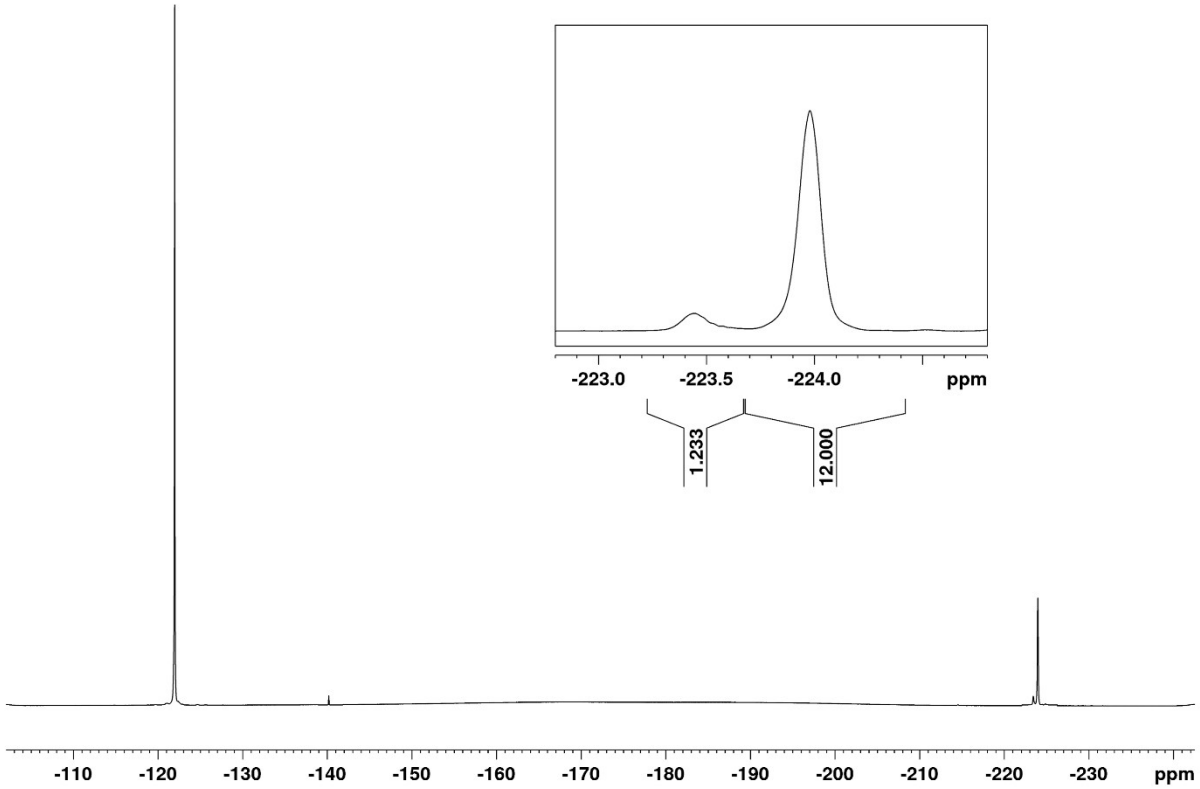


Figure S- 18: ^{19}F-NMR spectrum (282.45 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurity of 0.43 eq of C$_{10}$F$_{15}$OH.

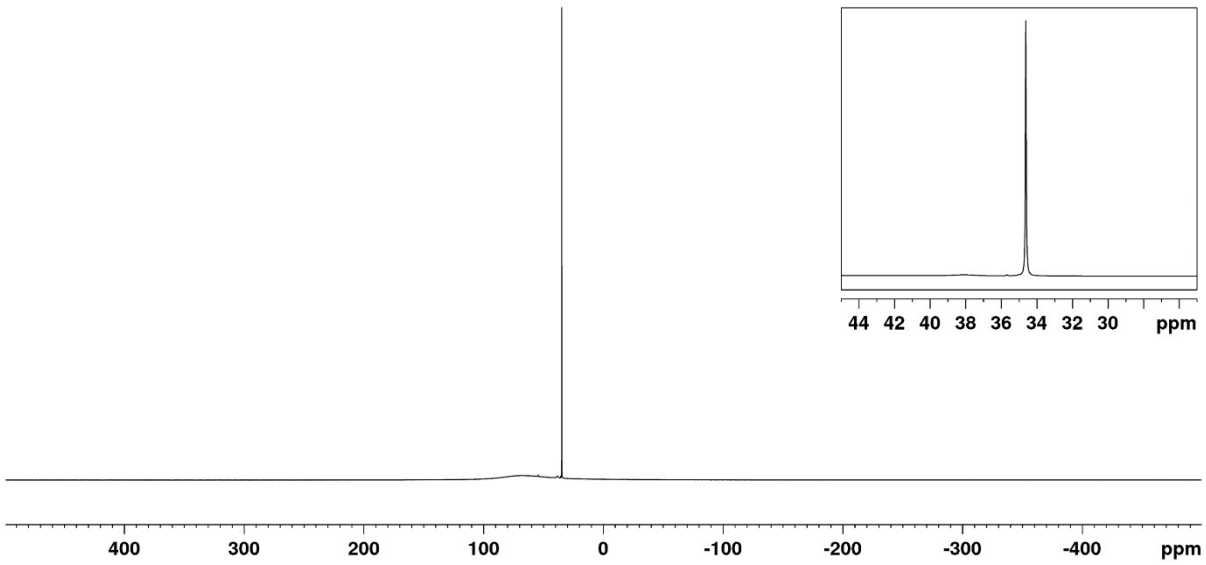


Figure S- 19: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$] containing impurity of 0.43 eq of C$_{10}$F$_{15}$OH.

Synthesis of Na[Al(OC$_{10}$F$_{15}$)$_4$] containing impurities of C$_{10}$F$_{15}$OH

Purified and slightly ground $NaAlH_4$ (0,033 g, 0.61 mmol) and perfluoro-1-adamantanol (1.074 g, 2.544 mmol, 4.16 eq) were submitted into a Schlenk flask and suspended in *o*-DFB (10 mL). The reaction mixture was stirred for two days under reflux and analyzed by NMR spectroscopy. The solvent

was removed under reduced pressure, washed with toluene (3x 5,0 mL) and dried in *vacuo* at 90°C. The obtained colorless solid (0.980 g, 0.565 mmol, 92,5 %) was analyzed by NMR spectroscopy showing impurity of unreacted alcohol $C_{10}F_{15}OH$ and and very small amounts of $[F{-}Al(OC_{10}F_{15})_3]^-$.

The NMR spectra of the reaction solution as well as the isolated solid show the identical resonances. Only of the reaction solution an additional $^{19}F,^{27}Al$-COSY spectrum was measured. Therefore, only the spectra of the reaction solution are presented.

^{1}H-NMR (300.18 MHz, 298 K, *o*-DFB/THF): δ = 9.52 (br. s, 1H, $C_{10}F_{15}O$**H**) ppm.
^{19}F-NMR (282.45 MHz, 298 K, *o*-DFB/THF): δ = −223.7 (m, C**F**, 12F, $Na[Al(OC_{10}F_{15})_4]$), −223.2 (m, C**F**, 3F, $C_{10}F_{15}OH$), −191.3 (m, **F**, 1F, $[\mathbf{F}{-}Al(OC_{10}F_{15})_3]^-$), −122.2 (m, C$\mathbf{F_2}$, 12F, $C_{10}F_{15}OH$), −121.7 (m, C$\mathbf{F_2}$, 48F, $Na[Al(OC_{10}F_{15})_4]$) ppm.
^{23}Na-NMR (79.40 MHz, 298 K, *o*-DFB/THF): δ = −6.5 (s, 1Na, **Na**$[Al(OC_{10}F_{15})_4]$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, *o*-DFB/THF): δ = 34.9 (s, 1Al, $Na[\mathbf{Al}(OC_{10}F_{15})_4]$), 42.5 (m, 1Al, $[F{-}Al(OC_{10}F_{15})_3]^-$) ppm.

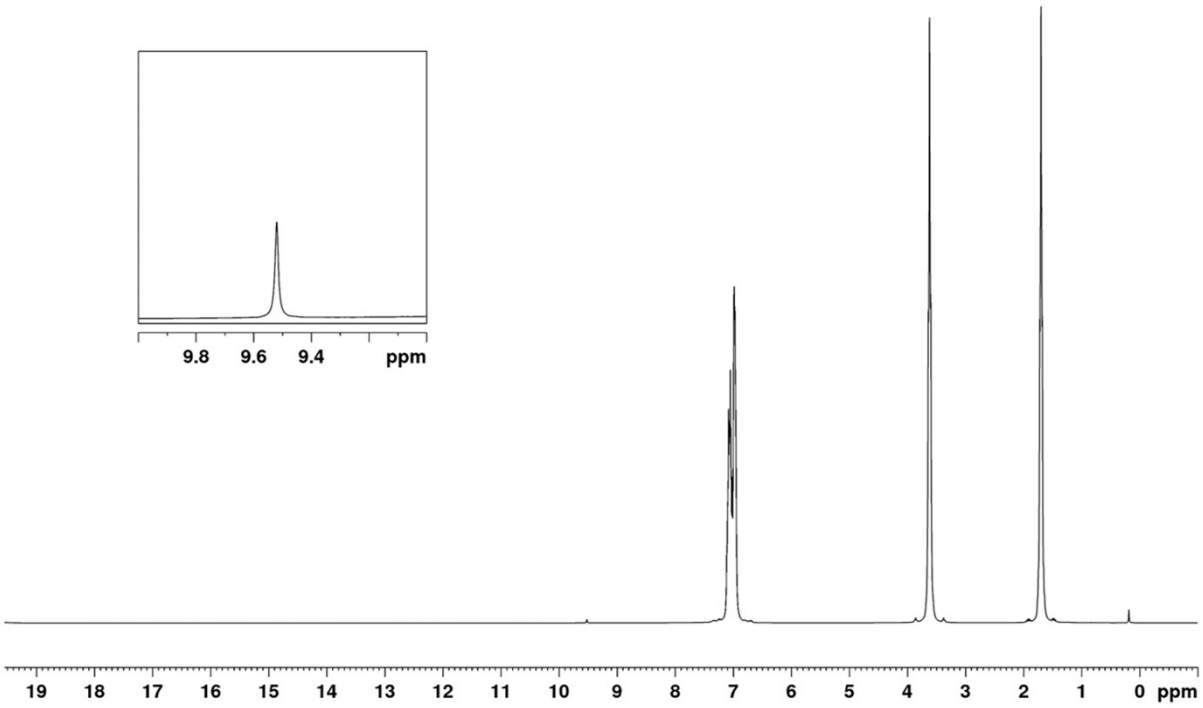


Figure S- 20: ^{1}H-NMR spectrum (300.18 MHz, 298 K, *o*-DFB/THF) of $Na[Al(OC_{10}F_{15})_4]$ of the reaction solution.

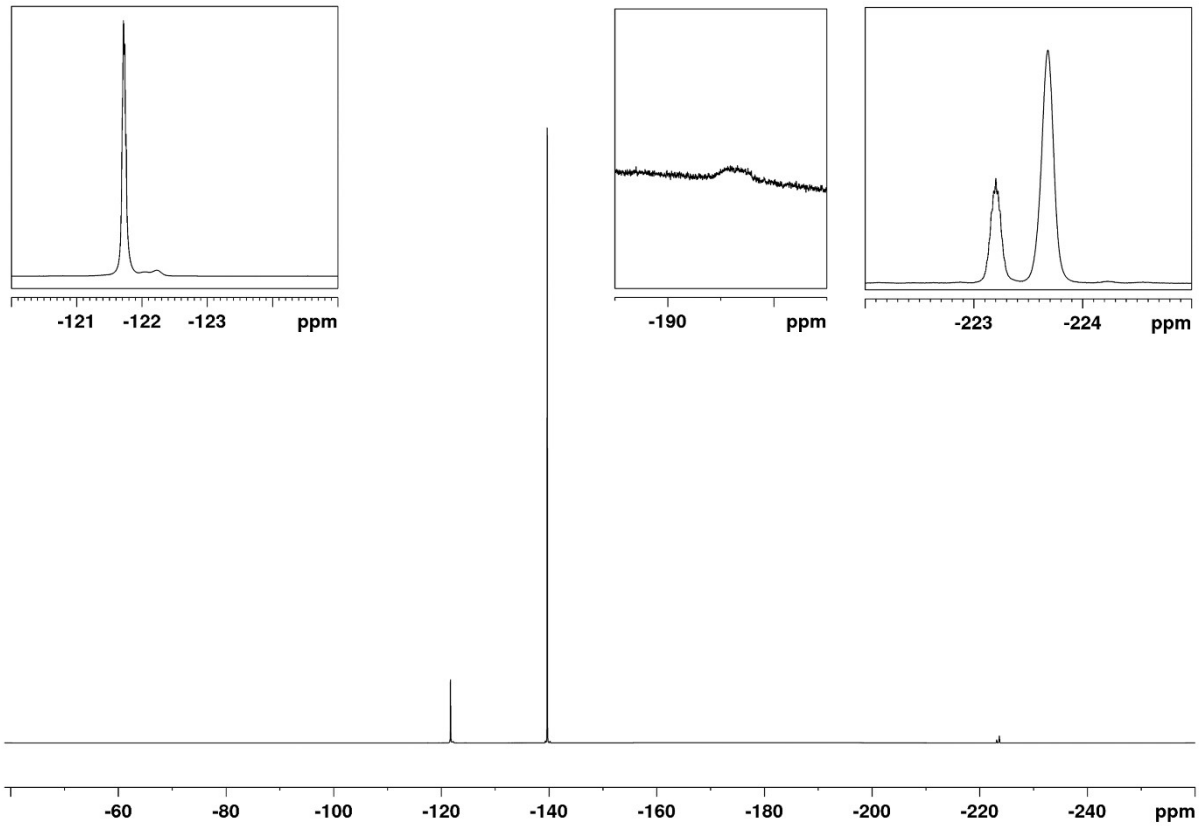


Figure S- 21: ^{19}F-NMR spectrum (282.45 MHz, 298 K, *o*-DFB/THF) of Na[Al($OC_{10}F_{15}$)$_4$] of the reaction solution.

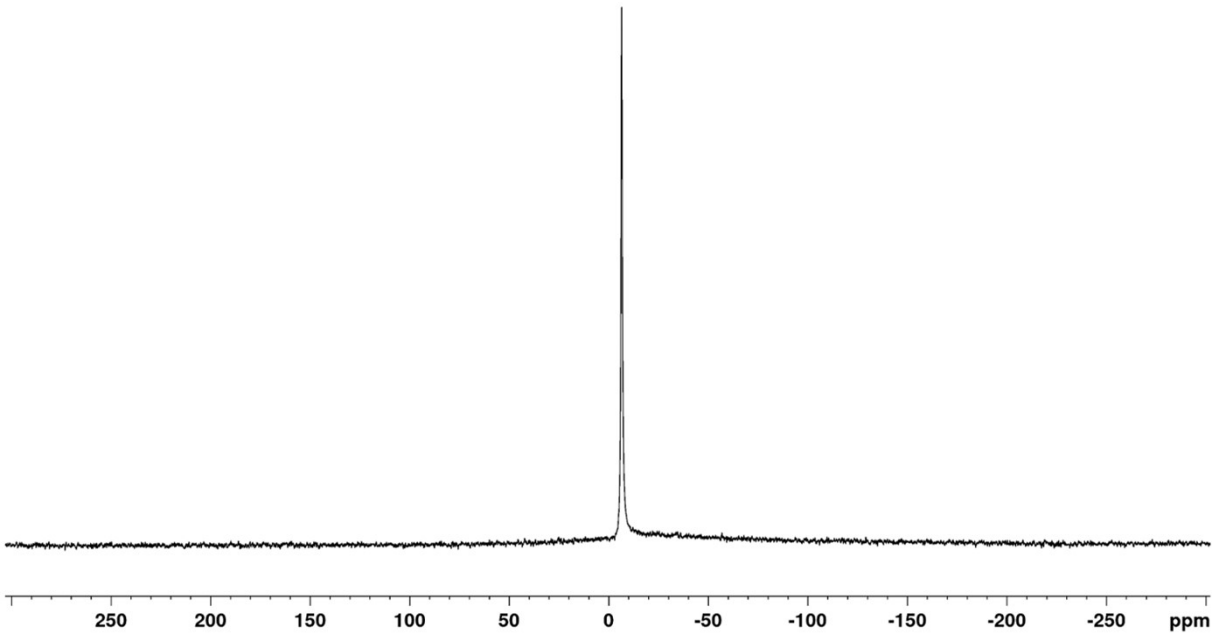


Figure S- 22: ^{23}Na-NMR spectrum (79.40 MHz, 298 K, *o*-DFB/THF) of Na[Al($OC_{10}F_{15}$)$_4$] of the reaction solution.

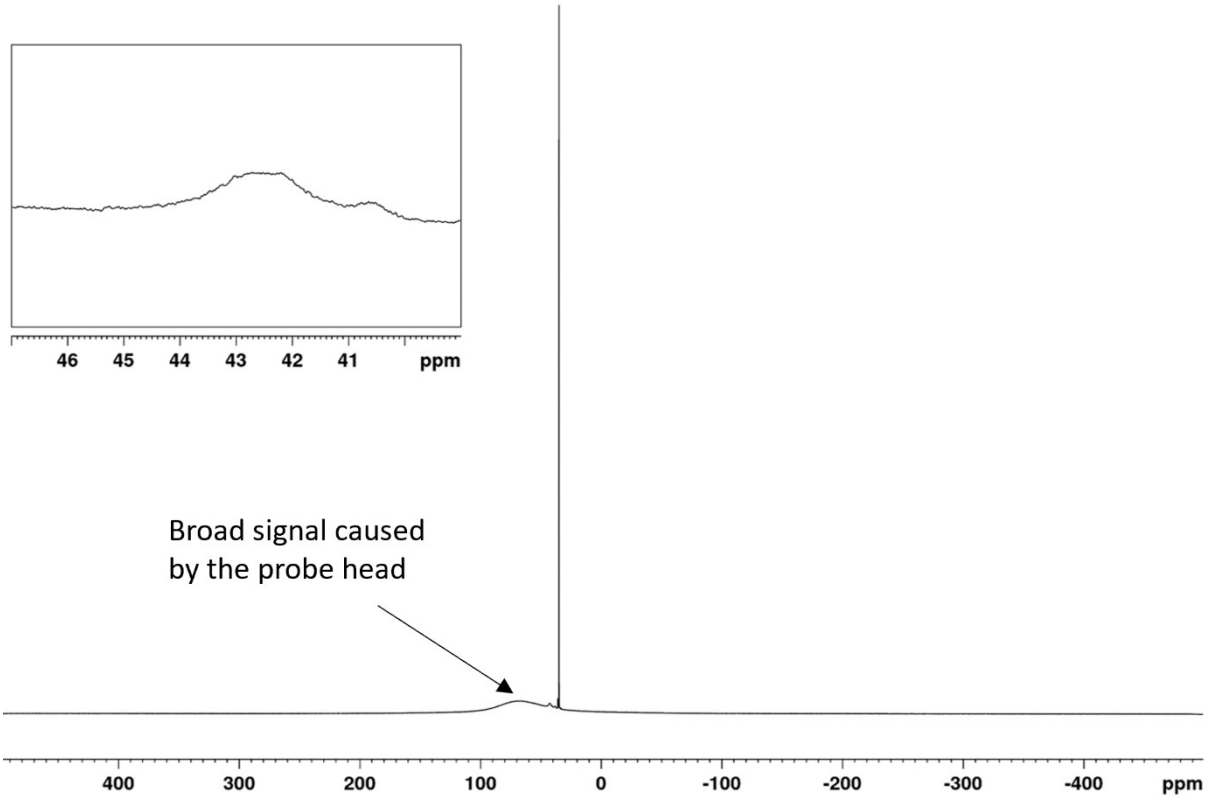


Figure S- 23: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, *o*-DFB/THF) of Na[Al($OC_{10}F_{15}$)$_4$] of the reaction solution.

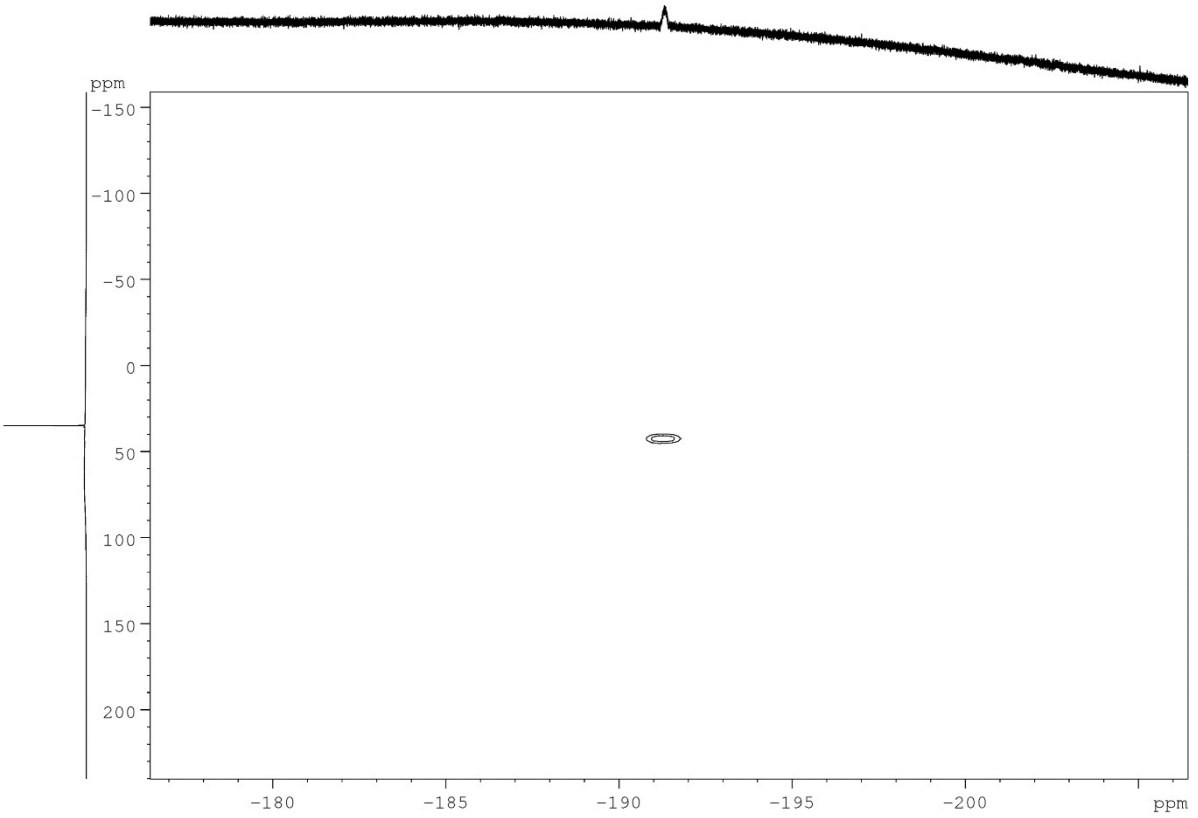


Figure S- 24: ^{19}F,^{27}Al-COSY-NMR spectrum (282.45 MHz, 78.22 MHz, 298 K, *o*-DFB/THF) of Na[Al($OC_{10}F_{15}$)$_4$] of the reaction solution.

Synthesis of $Ag[Al(OC_{10}F_{15})_4]$ containing impurities of $C_{10}F_{15}O^-$

$Li[Al(OC_{10}F_{15})_4]$ (0.205 g, 0.152 mmol) containing impurities of alcoholate $C_{10}F_{15}O^-$ (since this was one of the first attempts wherein the dried alcohol $C_{10}F_{15}OH$ was not sublimed prior to synthesis of $Li[Al(OC_{10}F_{15})_4]$ consequently containing $NaOC_{10}F_{15}$) and AgF (0.048 g, 0.378 mmol, 3.17 eq.) were suspended in *o*-DFB (5.0 mL) and sonicated for 14 h. After sedimentation of the solid an NMR was measured from the solution.

The reaction mixture was filtered and crystallized by diffusion crystallization with n-pentane (5 mL) for purification. The growth of two different sorts of suitable crystals for single crystal XRD was obtained in the form of colorless needles ($[Ag_3(OC_{10}F_{15})_2(o\text{-DFB})_3][Al(OC_{10}F_{15})_4]$) **3** and blocks ($[Ag(o\text{-DFB})_2][Al(OC_{10}F_{15})_4]$) **2-*o*DFB**. Since it was impossible to separate the two different sorts of crystals no declaration of yield is reasonable at this point. For further investigation, an NMR of the isolated crystals containing both sorts of crystals was measured in CH_2Cl_2. However, the NMR probe contained undissolved solid. After the NMR sample was measured, the solution was filtered off and the remaining solid dissolved in *o*-DFB and again analyzed by NMR spectroscopy.

NMR data of the reaction solution:

^{1}H-NMR (400.17 MHz, 298 K, CD_2Cl_2): δ = 7.19 (m, 4H, *o*-DFB) ppm.
^{7}Li-NMR (155.52 MHz, 298 K, CD_2Cl_2): no signal (as expected)
^{19}F-NMR (376.54 MHz, 298 K, CD_2Cl_2): δ = −223.3 (m, C**F**, 12F, $Ag[Al(OC_{10}F_{15})_4]$), −222.4 (m, C**F**, 3F, $AgOC_{10}F_{15}$), −139.4 (m, 2F, o-DFB), −122.6 (m, C**F_2**, 12F, $AgOC_{10}F_{15}$), −121.6 (m, C**F_2**, 48F, $Ag[Al(OC_{10}F_{15})_4]$) ppm.
^{27}Al-NMR (104.27 MHz, 298 K, CD_2Cl_2): δ = 35.0 (s, 1Al, $Ag[$**Al**$(OC_{10}F_{15})_4]$) ppm.

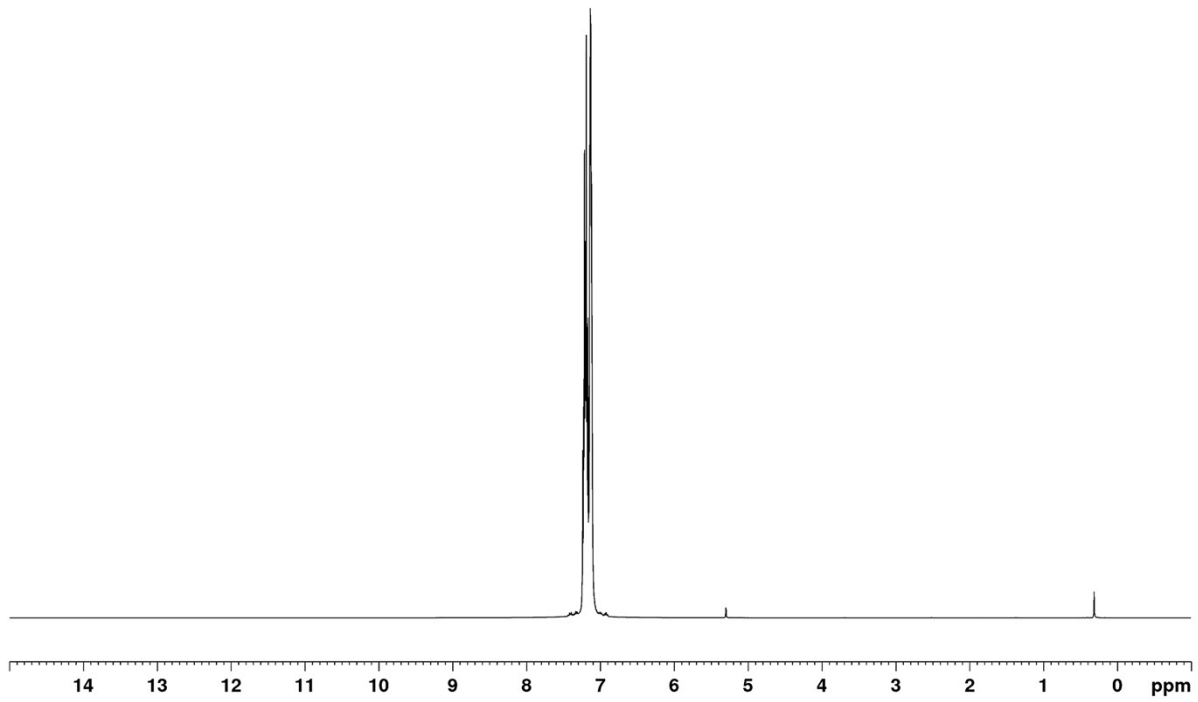


Figure S- 25: ^{1}H-NMR spectrum (400.17 MHz, 298 K, CD_2Cl_2) of $Ag[Al(OC_{10}F_{15})_4]$ of the reaction solution.

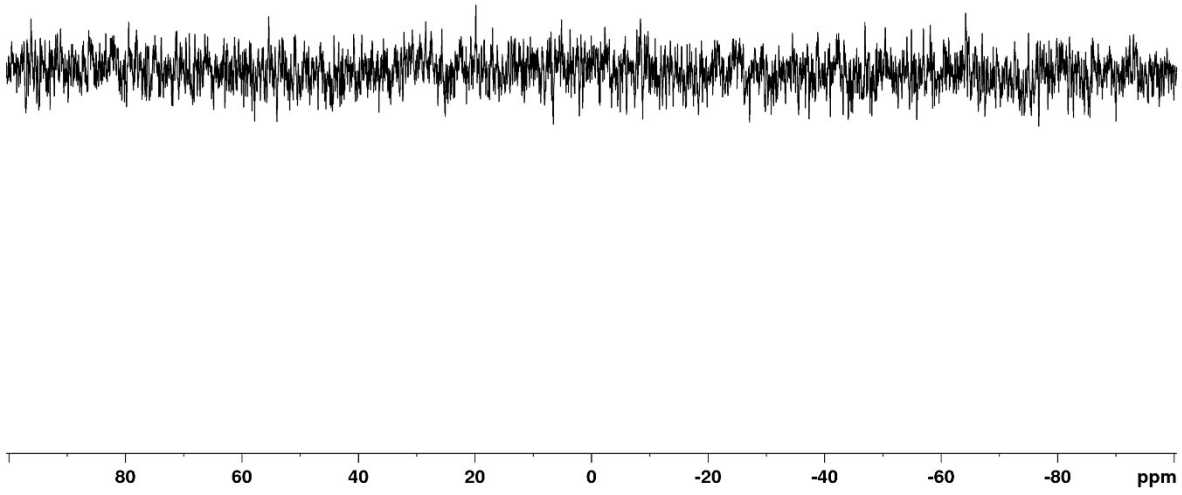


Figure S- 26: ^{7}Li-NMR spectrum (155.52 MHz, 298 K, CD_2Cl_2) of $Ag[Al(OC_{10}F_{15})_4]$ of the reaction solution.

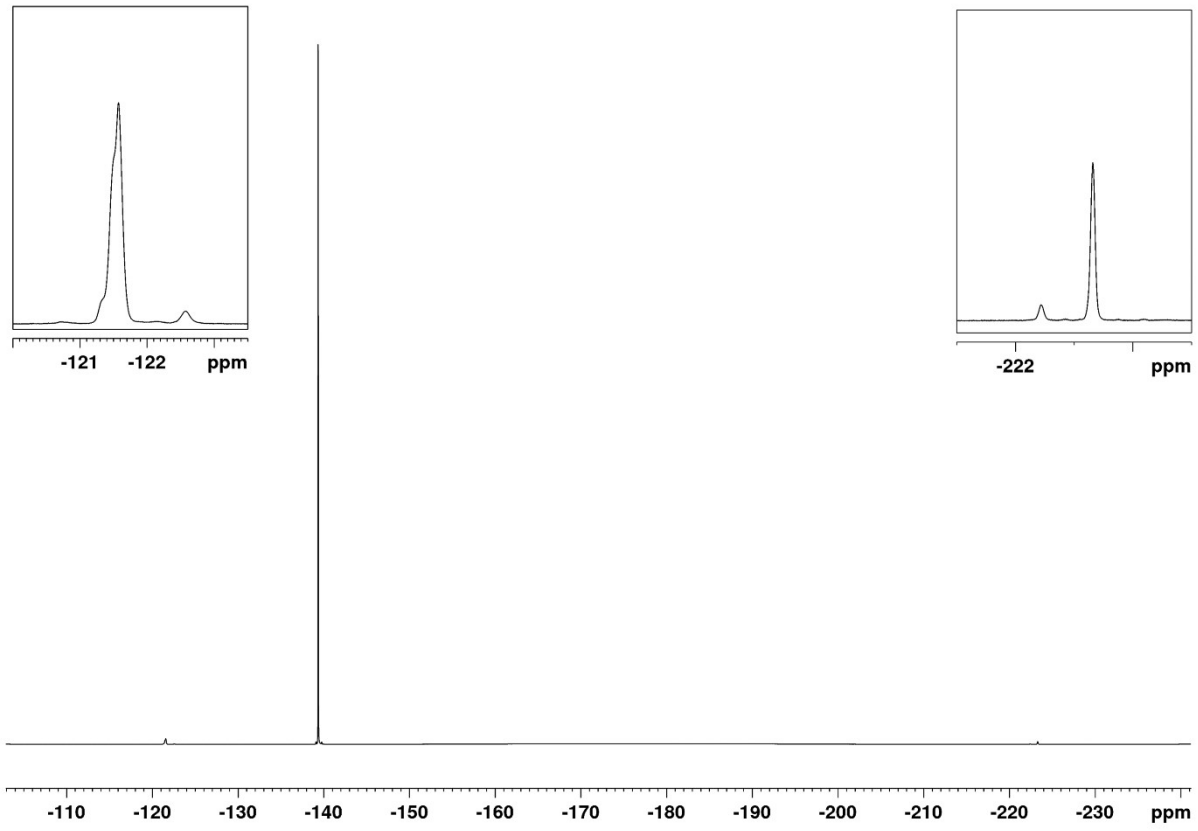


Figure S- 27: ^{19}F-NMR spectrum (376.54 MHz, 298 K, CD_2Cl_2) of $Ag[Al(OC_{10}F_{15})_4]$ of the reaction solution.

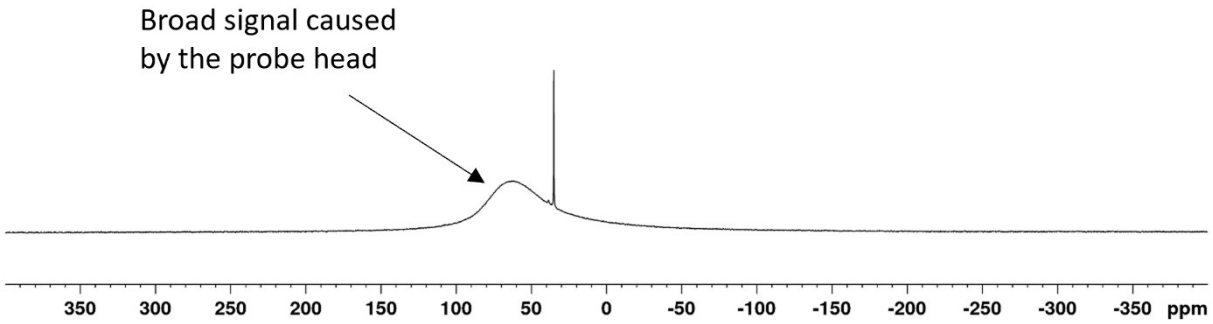


Figure S- 28: ^{27}Al-NMR spectrum (104.27 MHz, 298 K, CD_2Cl_2) of $Ag[Al(OC_{10}F_{15})_4]$ of the reaction solution.

NMR data of the isolated crystals in CH_2Cl_2:

^{1}H-NMR (300.18 MHz, 298 K, CH_2Cl_2): δ = 7.16 (m, 4H, *o*-DFB) ppm.
^{7}Li-NMR (116.66 MHz, 298 K, CH_2Cl_2): no signal (as expected)
^{19}F-NMR (282.45 MHz, 298 K, CH_2Cl_2): δ = −223.4 (m, C**F**, 12F, $Ag[Al(OC_{10}F_{15})_4]$), −139.4 (m, 2F, o-DFB), −122.0 (m, C**F_2**, $Ag[Al(OC_{10}F_{15})_4]$), −121.6 (m, C**F_2**, $Ag[Al(OC_{10}F_{15})_4]$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, CH_2Cl_2): δ = 34.7 (s, 1Al, $Ag[$**Al**$(OC_{10}F_{15})_4]$) ppm.

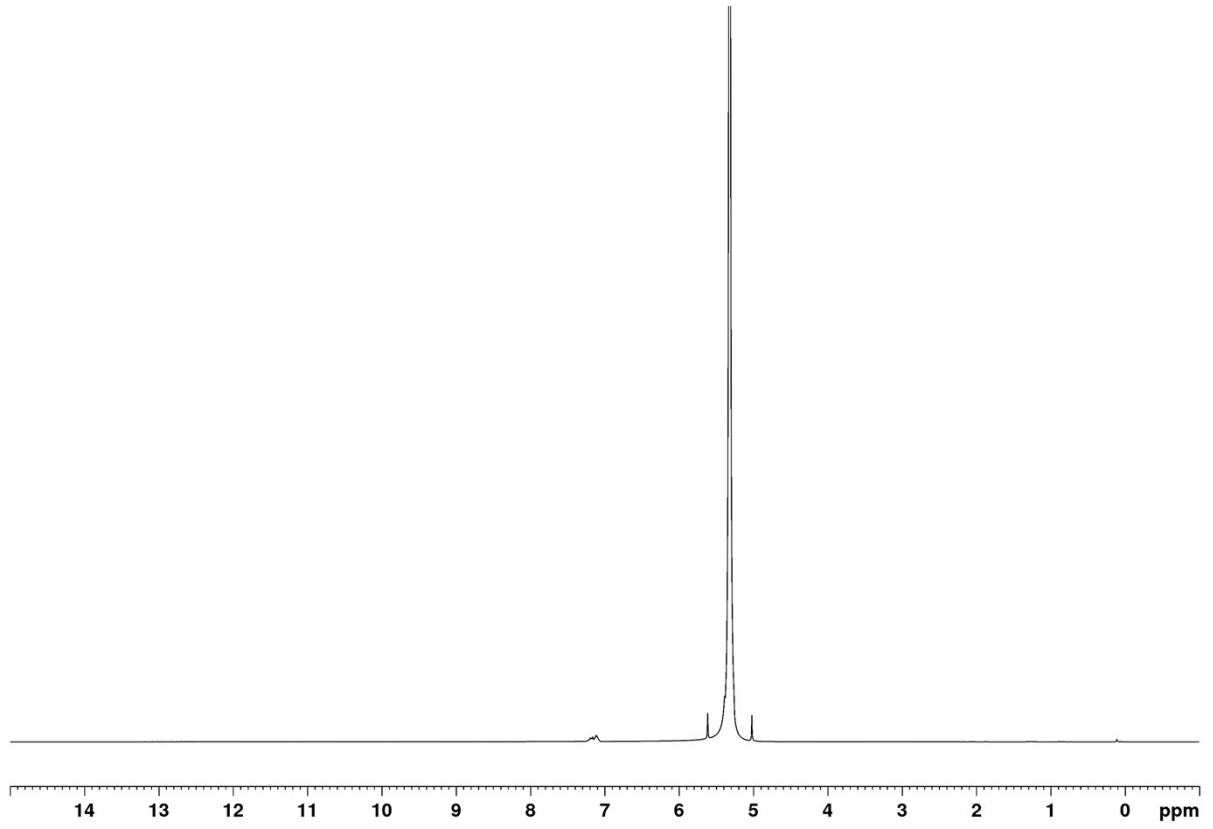


Figure S- 29: ^{1}H-NMR (300.18 MHz, 298 K, CH_2Cl_2) of $Ag[Al(OC_{10}F_{15})_4]$ of the isolated crystals containing undissolved solid.

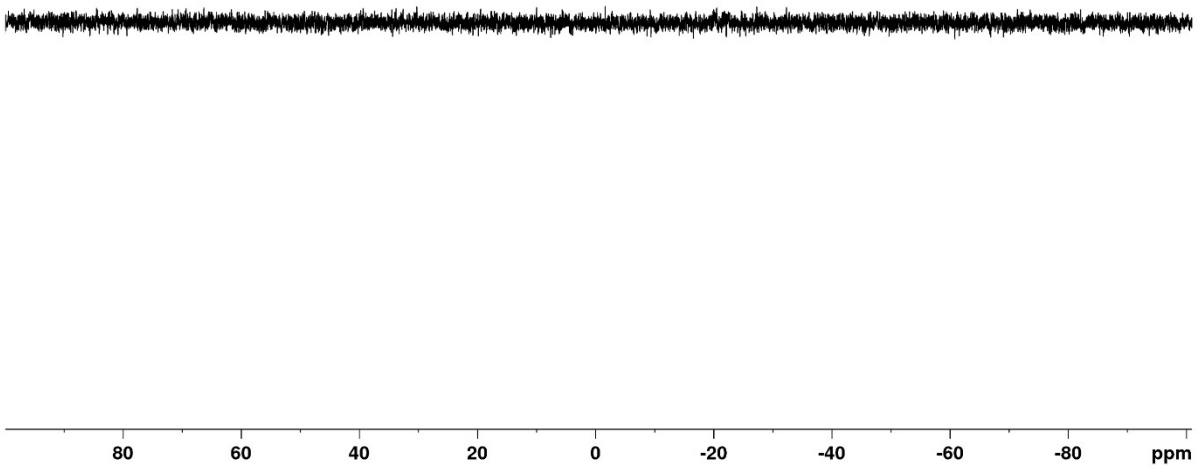


Figure S- 30: ^{7}Li-NMR (116.66 MHz, 298 K, CH_2Cl_2) of $Ag[Al(OC_{10}F_{15})_4]$ of the isolated crystals containing undissolved solid.

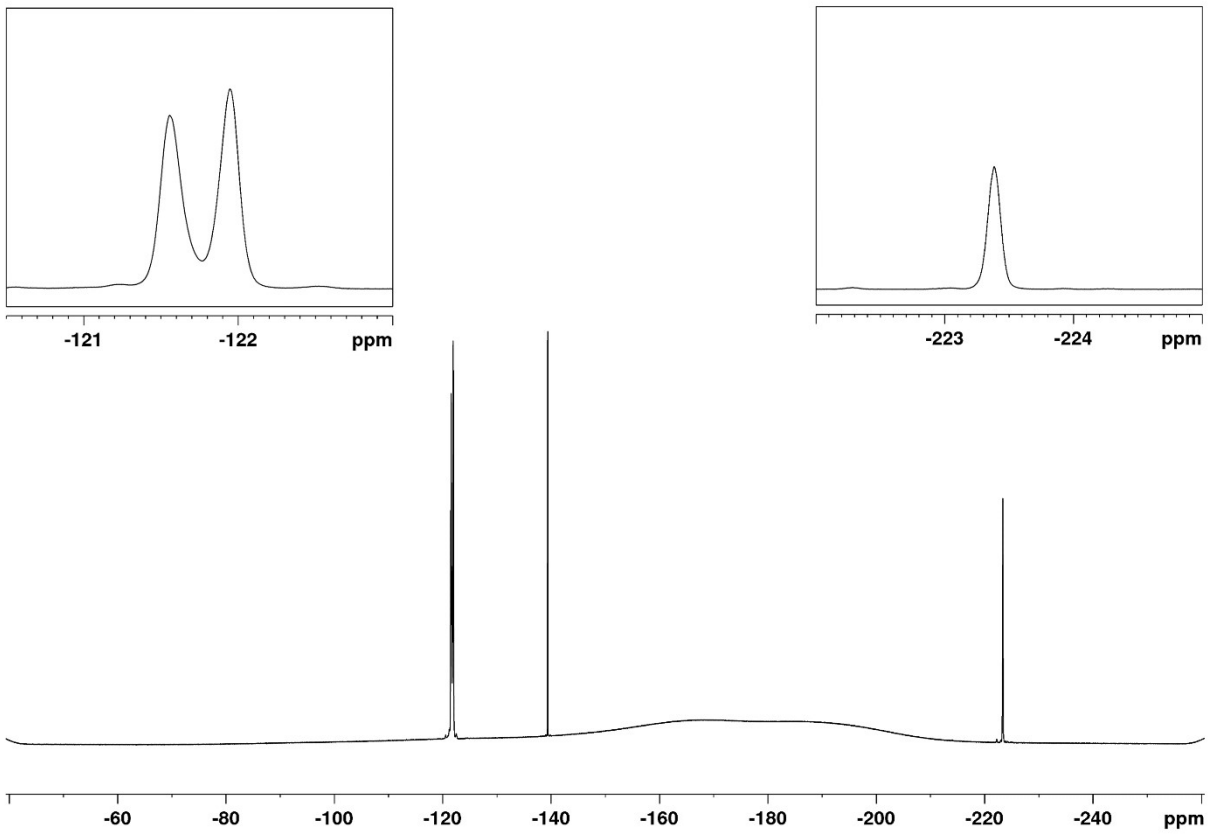


Figure S- 31: ^{19}F-NMR (282.45 MHz, 298 K, CH_2Cl_2) of $Ag[Al(OC_{10}F_{15})_4]$ of the isolated crystals containing undissolved solid.

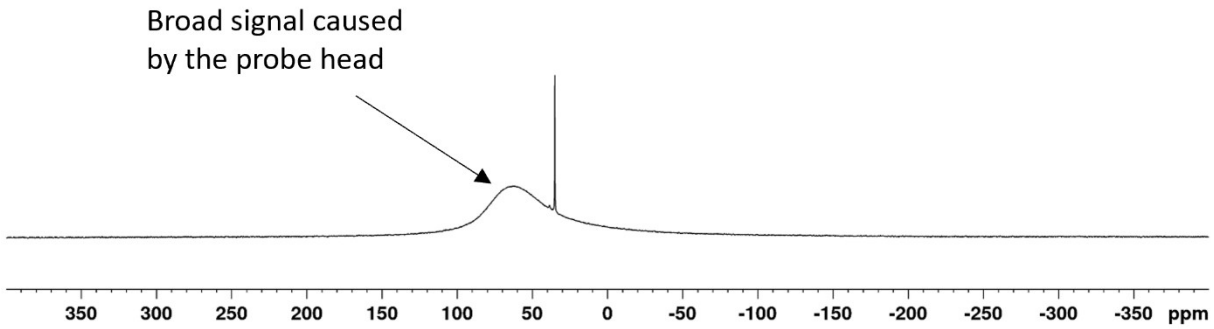


Figure S- 32: ^{27}Al-NMR (78.22 MHz, 298 K, CH_2Cl_2) of $Ag[Al(OC_{10}F_{15})_4]$ of the isolated crystals containing undissolved solid.

NMR data of the isolated in CH_2Cl_2 insoluble solid dissolved in *o*-DFB after filtration:

^{1}H-NMR (400.17 MHz, 298 K, *o*-DFB): δ = 5.26 (m, 2H, CH_2Cl_2) ppm.
^{7}Li-NMR (155.52 MHz, 298 K, *o*-DFB): was not measured.
^{19}F-NMR (376.54 MHz, 298 K, *o*-DFB): δ = −223.2 (m, C**F**, 12F, $[Al(OC_{10}F_{15})_4]^-$), −222.4 (m, C**F**, 3F, $C_{10}F_{15}O^-$), −122.0 (m, C**F_2**, $Ag[Al(OC_{10}F_{15})_4]$), −121.6 (m, C**F_2**, $Ag[Al(OC_{10}F_{15})_4]$) ppm.
^{27}Al-NMR (104.27 MHz, 298 K, *o*-DFB): δ = 35.3 (s, 1Al, Ag[**Al**$(OC_{10}F_{15})_4$]) ppm.

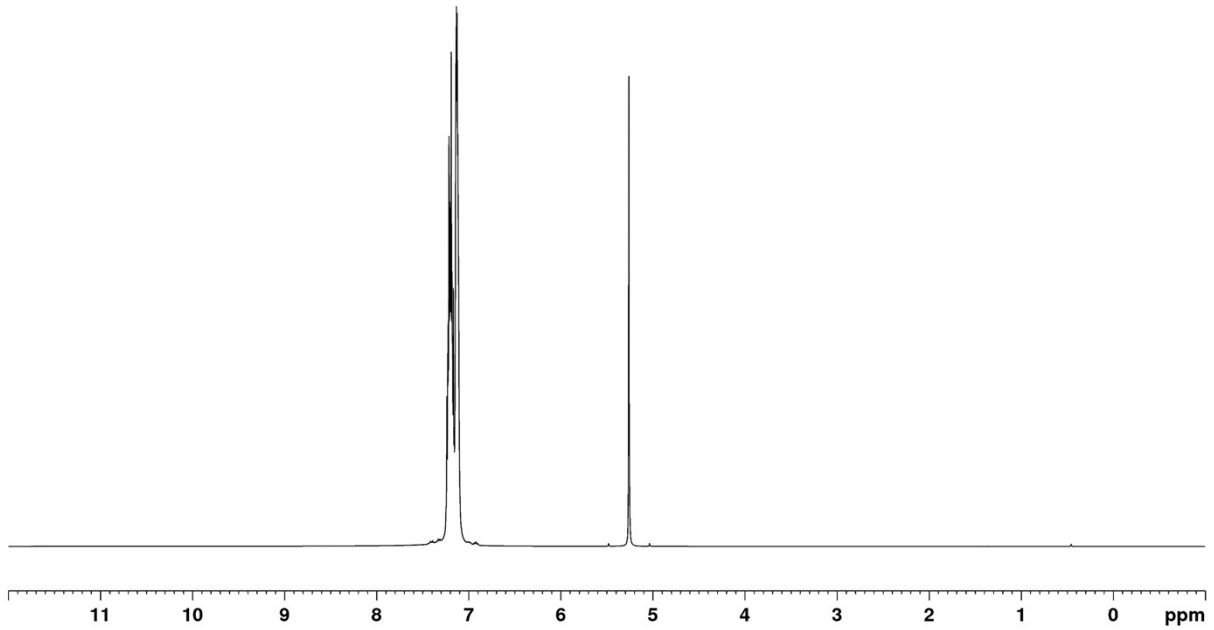


Figure S- 33: ^{1}H-NMR (400.17 MHz, 298 K, *o*-DFB) of $Ag[Al(OC_{10}F_{15})_4]$ of the in *o*-DFB dissolved solid.

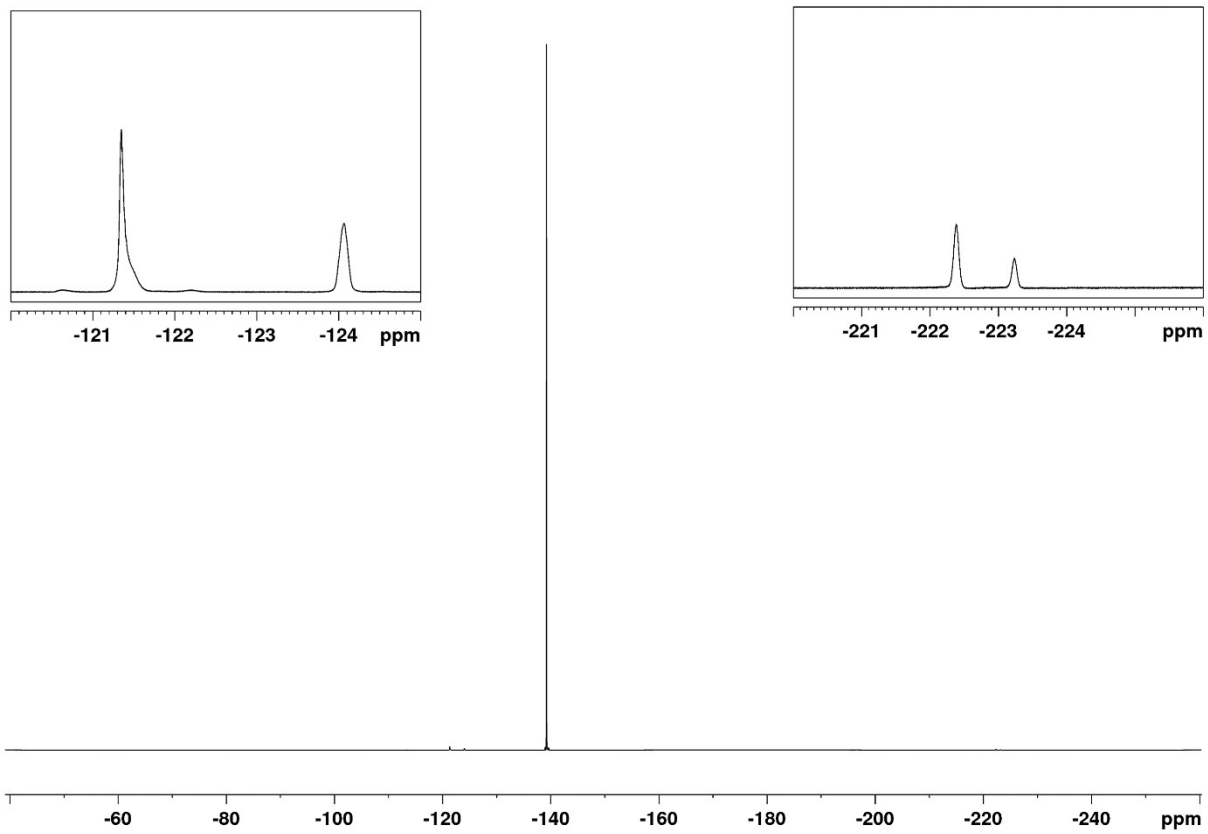


Figure S- 34: ^{19}F-NMR (376.54 MHz, 298 K, *o*-DFB) of Ag[Al(OC$_{10}$F$_{15}$)$_4$] of the in *o*-DFB dissolved solid.

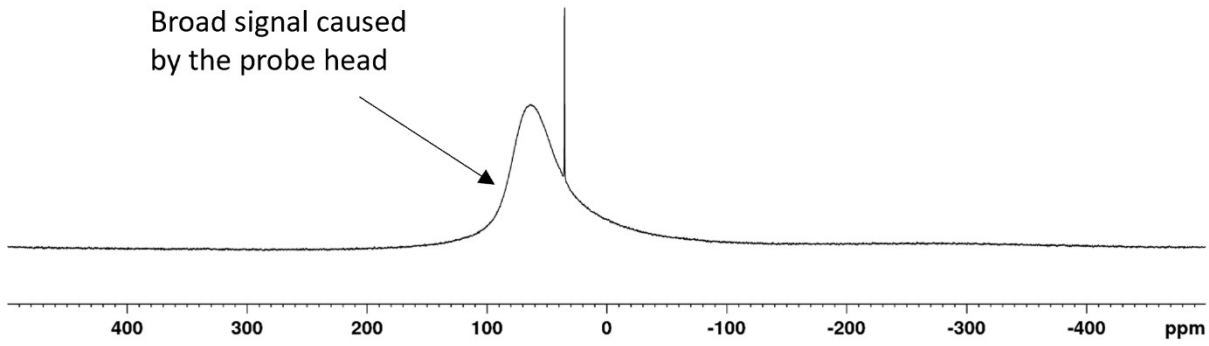


Figure S- 35: ^{27}Al-NMR (104.27 MHz, 298 K, *o*-DFB) of Ag[Al(OC$_{10}$F$_{15}$)$_4$] of the in *o*-DFB dissolved solid.

Synthesis of $Ag(CH_2Cl_2)_2[Al(OC_{10}F_{15})_4]$

$Li[Al(OC_{10}F_{15})_4]$ (0.855 g, 0.498 mmol) containing impurities of alcohol $C_{10}F_{15}OH$ and AgF (0.104 g, 0.820 mmol, 1.65 eq) were suspended in *o*-DFB (3.0 mL) and sonicated for 10 h. The solvent *o*-DFB was removed under reduced pressure. CH_2Cl_2 (3.0 mL) was added, and the target compound extracted 5x by condensing the solvent back to the reaction mixture after filtration. *n*-pentane was added into the empty part of the H-cell (where the reaction took place) for diffusion crystallization. The target compound was obtained as colorless crystals (0.360 g, 0.200 mmol, 40 %), washed with *n*-pentane (2x 5 mL), dried under reduced pressure, and analyzed by NMR and IR spectroscopy.

^{1}H-NMR (300.18 MHz, 298 K, CD_2Cl_2): δ = 5.32 (s, 2H, C**H_2**Cl_2) ppm.
^{7}Li-NMR (116.66 MHz, 298 K, CD_2Cl_2): no signal (as expected)
^{19}F-NMR (282.45 MHz, 298 K, CD_2Cl_2): δ = −223.4 (m, C**F**, 12F, $Ag[Al(OC_{10}F_{15})_4]$), −122.0 (m, C**F_2**, $Ag[Al(OC_{10}F_{15})_4]$), −121.6 (m, C**F_2**, $Ag[Al(OC_{10}F_{15})_4]$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, CD_2Cl_2): δ = 34.7 (s, 1Al, $Ag[$**Al**$(OC_{10}F_{15})_4]$) ppm.
FTIR (Diamant, ATR): $\tilde{\nu}$ = 2966 (vw), 1351 (vw), 1268 (vs), 1106 (vw), 1038 (vw), 981 (m), 955 (vs), 852 (vw), 814 (vw), 758 (vw), 736 (vw), 679 (vw), 651 (vw), 533 (vw), 442 (vw), 402 cm^{-1}.

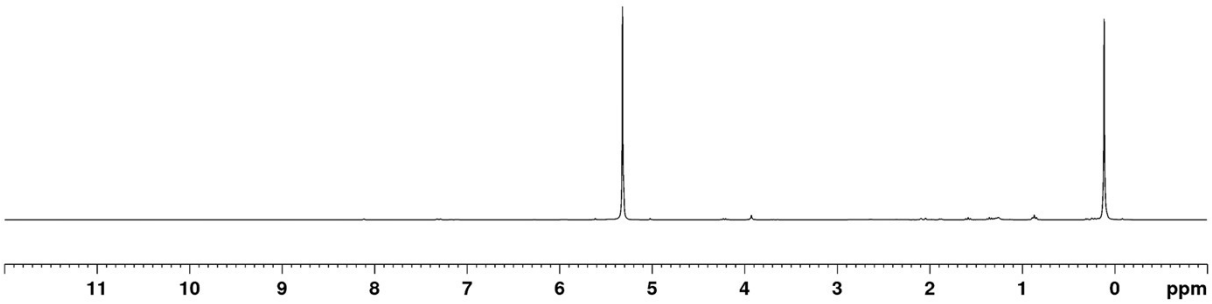


Figure S- 36: ^{1}H-NMR (300.18 MHz, 298 K, CD_2Cl_2) of isolated crystals of $Ag(CH_2Cl_2)_2[Al(OC_{10}F_{15})_4]$.

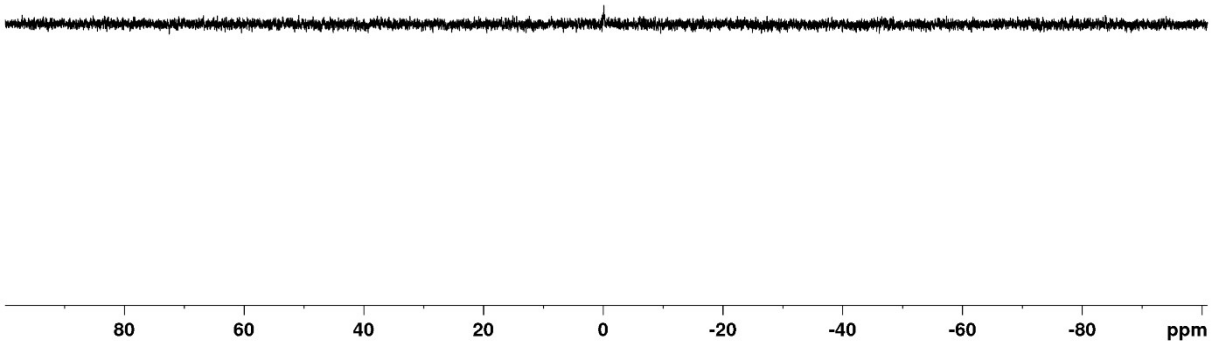


Figure S- 37: ^{7}Li-NMR (116.66 MHz, 298 K, CD_2Cl_2) of isolated crystals of $Ag(CH_2Cl_2)_2[Al(OC_{10}F_{15})_4]$.

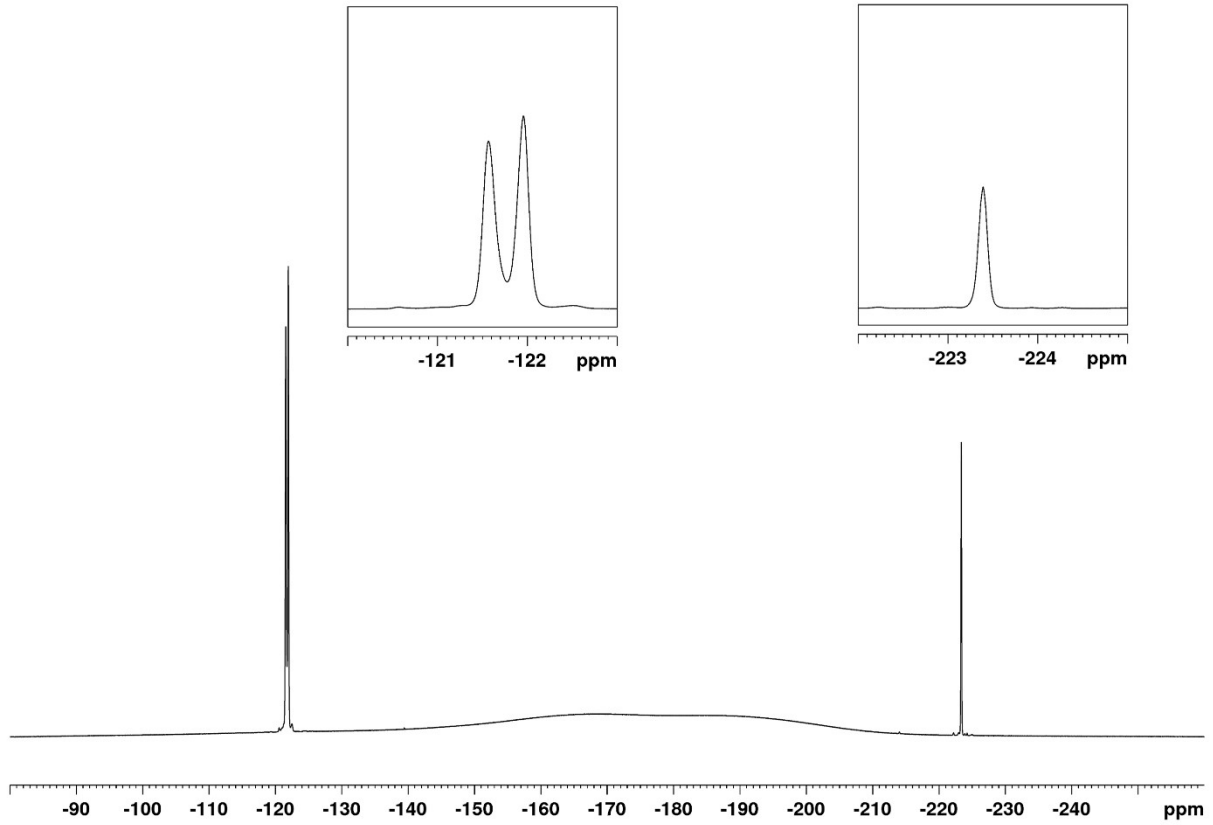


Figure S- 38: ^{19}F-NMR (282.45 MHz, 298 K, CD_2Cl_2) of isolated crystals of $Ag(CH_2Cl_2)_2[Al(OC_{10}F_{15})_4]$.

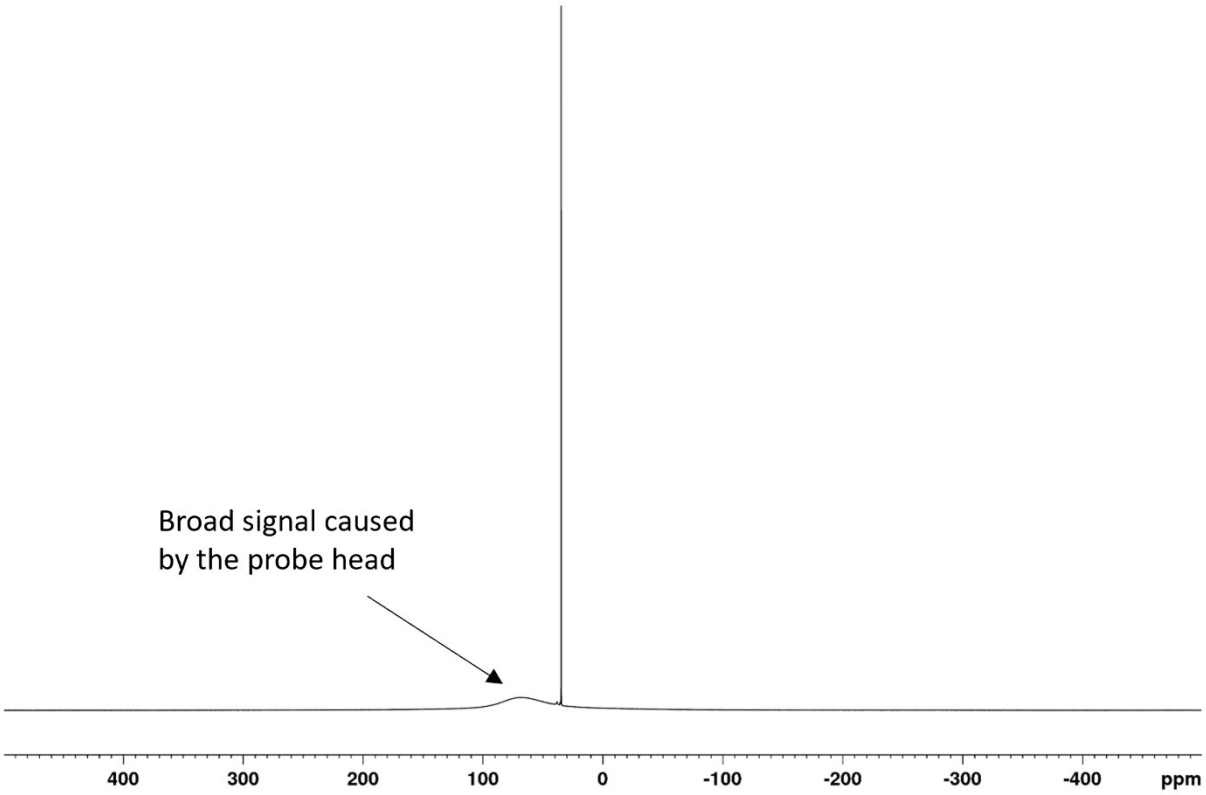


Figure S- 39: ^{27}Al-NMR (78.22 MHz, 298 K, CD_2Cl_2) of isolated crystals of $Ag(CH_2Cl_2)_2[Al(OC_{10}F_{15})_4]$.

The amount of coordinated CH_2Cl_2 towards Ag^+ even after drying was calculated by NMR spectroscopy. For this purpose, the NMR signals of the anion in the ^{19}F-NMR spectrum were referenced to added *o*-DFB and compared to the integrals of CH_2Cl_2 in the ^{1}H-NMR spectrum, as followed:

^{1}H-NMR spectrum: Integral of *o*-DFB : 4 -> 1; integral of CH_2Cl_2 : 2 -> 0.103. Consequently, the stoichiometric ratio *o*-DFB : CH_2Cl_2 amounts to 1.0 : 0.1

^{19}F-NMR spectrum: Integral of *o*-DFB : 2 -> 1, integral of anion resonances with chemical shifts of −122.0 and −121.6 ppm (4x6x CF_2): 2.16 : 48 -> 0.05. Consequently, the stoichiometric ratio *o*-DFB : anion amounts to 1.0 : 0.05

Finally, the ratio of CH_2Cl_2 : anion contains 0.1 : 0.05 -> 2 : 1.

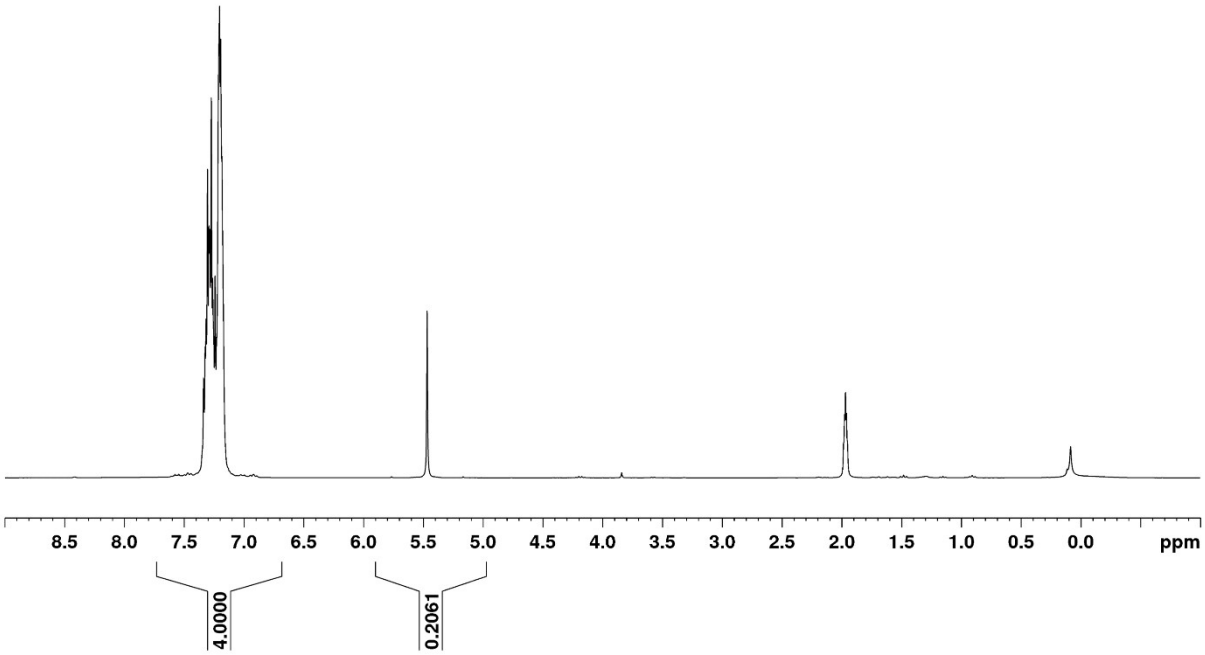


Figure S- 40: ^{1}H-NMR (300.18 MHz, 298 K, CD_3CN/*o*-DFB) of isolated crystals of $Ag(CH_2Cl_2)_2[Al(OC_{10}F_{15})_4]$ for quantification of the amount of CH_2Cl_2 coordinated towards Ag^+.

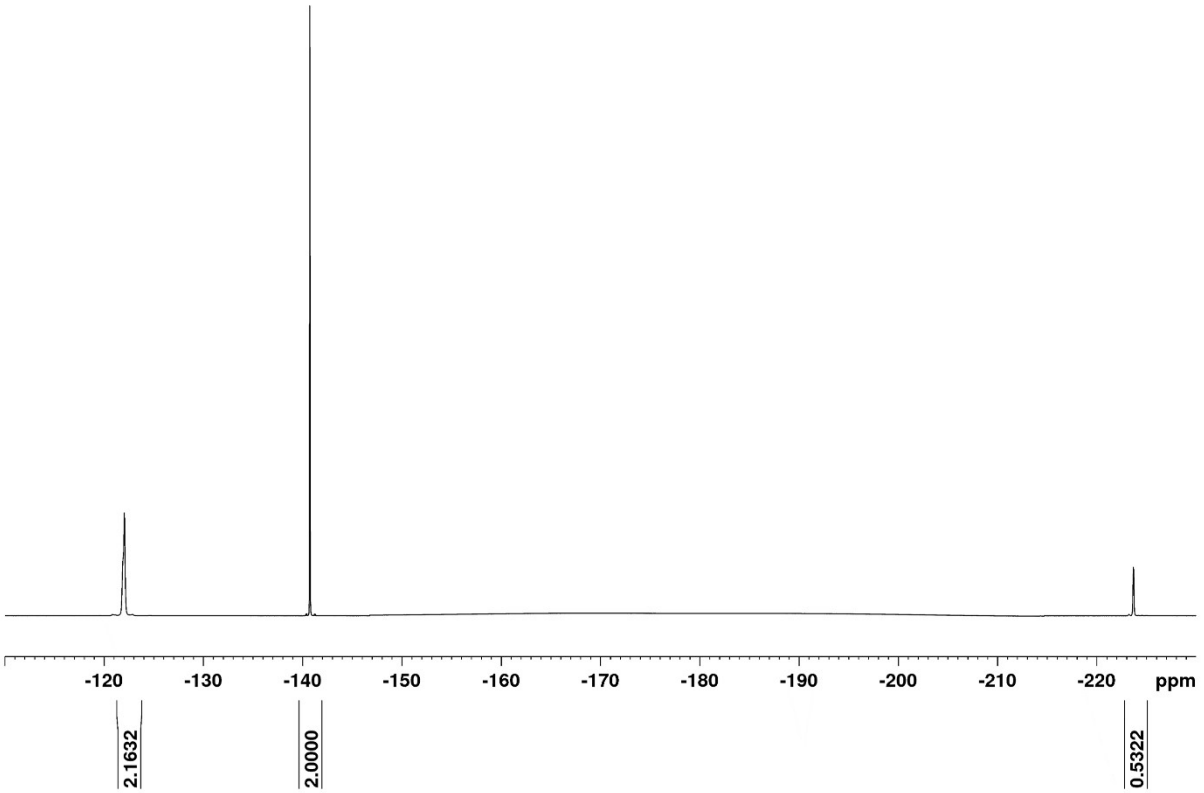


Figure S- 41: ^{19}F-NMR (282.45 MHz, 298 K, CD_3CN/*o*-DFB) of isolated crystals of $Ag(CH_2Cl_2)_2[Al(OC_{10}F_{15})_4]$ for quantification of the amount of CH_2Cl_2 coordinated towards Ag^+.

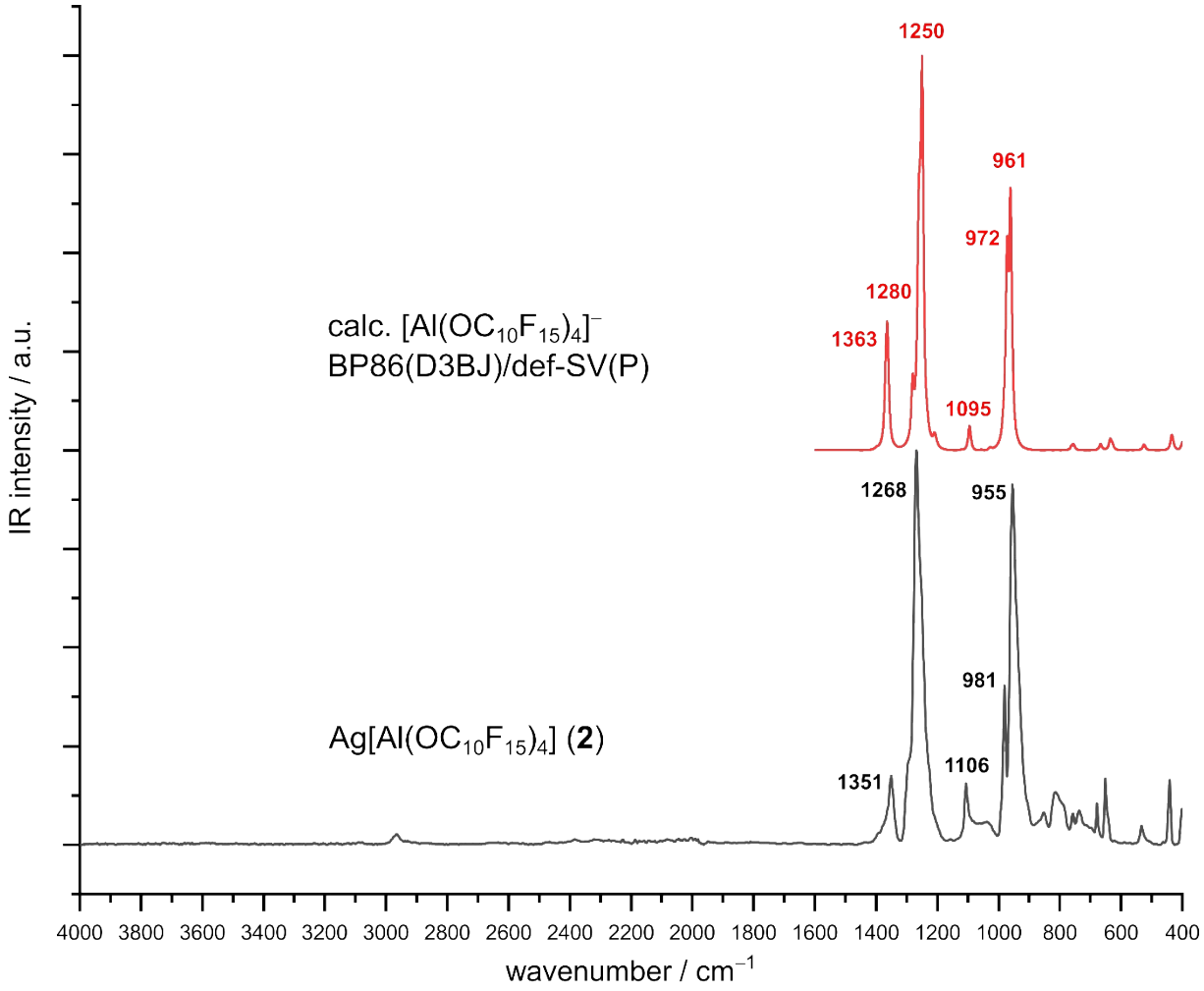


Figure S- 42: IR spectrum of $Ag(CH_2Cl_2)_2[Al(OC_{10}F_{15})_4]$ (black) in comparison with the calculated IR spectrum of the [*pfAd*]$^-$ anion at BP86(D3BJ)/def-SV(P) level of theory (red). All IR data of obtained pure substances of the [*pfAd*]$^-$ anion are compared and assigned in Table S- 1.

Synthesis of low yield $[Ph_3C][Al(OC_{10}F_{15})_4]$ containing impurities of $C_{10}F_{15}OH$

$Li[Al(OC_{10}F_{15})_4]$ (0.101 g, 0.059 mmol) containing impurities of alcohol $C_{10}F_{15}OH$ and Ph_3CCl (0.016 g, 0.057 mmol, 0.98 eq.) were suspended in CH_2Cl_2 (2.0 mL) and stirred at room temperature for two days. The reaction mixture was allowed to sediment and an NMR of the supernatant solution was measured. The solution was separated by filtration, the solid residue washed with CH_2Cl_2 (1.0 mL) and filtered again. Yellow crystals of the target (0.003 g, 0.002 mmol, 2.7 %) compound were isolated after diffusion crystallization with n-pentane. The obtained crystals were analyzed by single crystal X-ray diffraction and NMR spectroscopy.

NMR data of the reaction solution before crystallization:

^{1}H-NMR (300.18 MHz, 298 K, CD_2Cl_2): δ = 4.04 (br. s, 1H, $C_{10}F_{15}OH$), 7.12 (m, 2H, *o*-DFB), 7.29 (m, 2H, *o*-DFB), 7.68 (d, *o*-CH, 6H $[Ph_3C][Al(OC_{10}F_{15})_4]$, 7.91 (t, *m*-CH, 6H $[Ph_3C][Al(OC_{10}F_{15})_4]$), 8.30 (t, *p*-CH, 3H $[Ph_3C][Al(OC_{10}F_{15})_4]$) ppm.

^{7}Li-NMR (116.66 MHz, 298 K, CD_2Cl_2): no signal (as expected)

^{19}F-NMR (282.45 MHz, 298 K, CD_2Cl_2): δ = −223.4 (m, C**F**, 12F, $[Ph_3C][Al(OC_{10}F_{15})_4]$), −222.4 (m, C**F**, 3F, $C_{10}F_{15}OH$), −139.4 (m, 2F, *o*-DFB), −121.8 (m, C**F$_2$**, 48F, $[Ph_3C][Al(OC_{10}F_{15})_4]$), −121.1 (m, C**F**, 12F, $C_{10}F_{15}OH$) ppm.

^{27}Al-NMR (78.22 MHz, 298 K, CD_2Cl_2): δ = 34.7 (s, 1Al, $[Ph_3C][\mathbf{Al}(OC_{10}F_{15})_4]$) ppm.

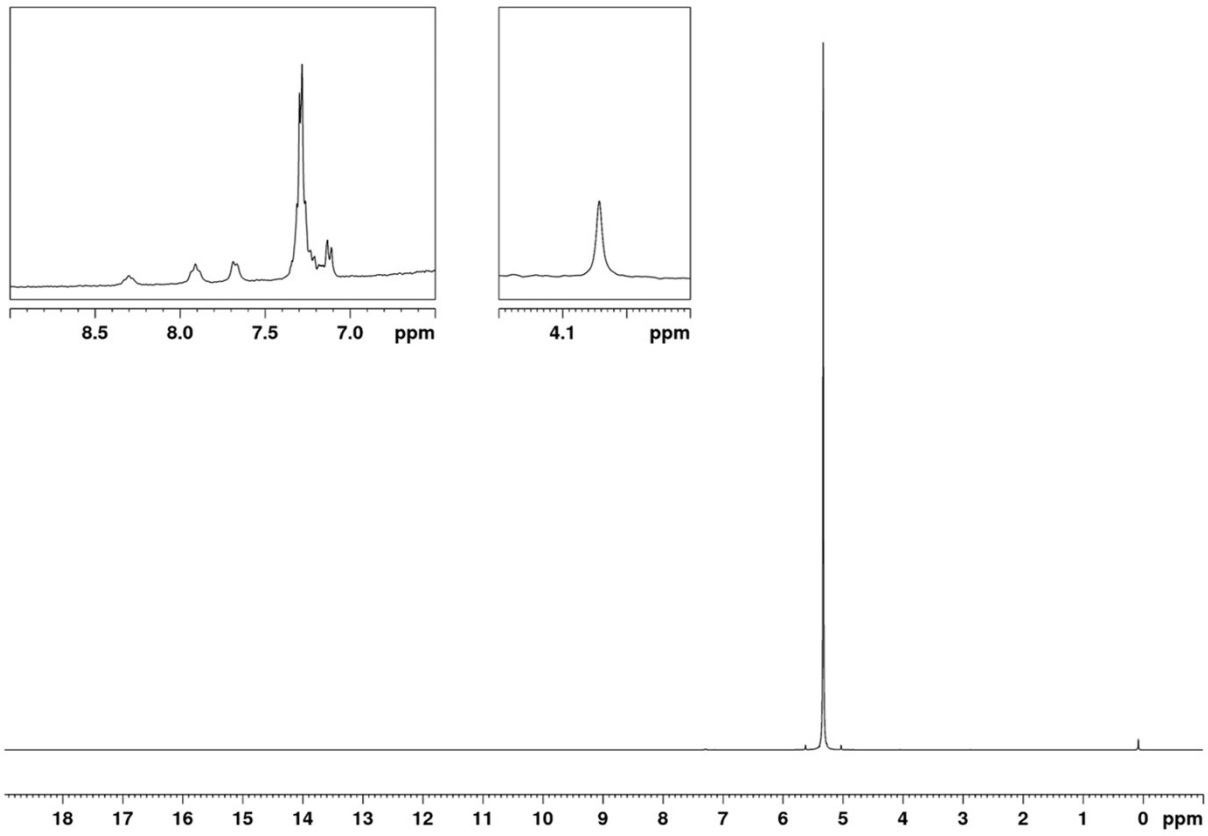


Figure S- 43: ^{1}H-NMR spectrum (300.18 MHz, 298 K, CD_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the reaction solution after sedimentaion.

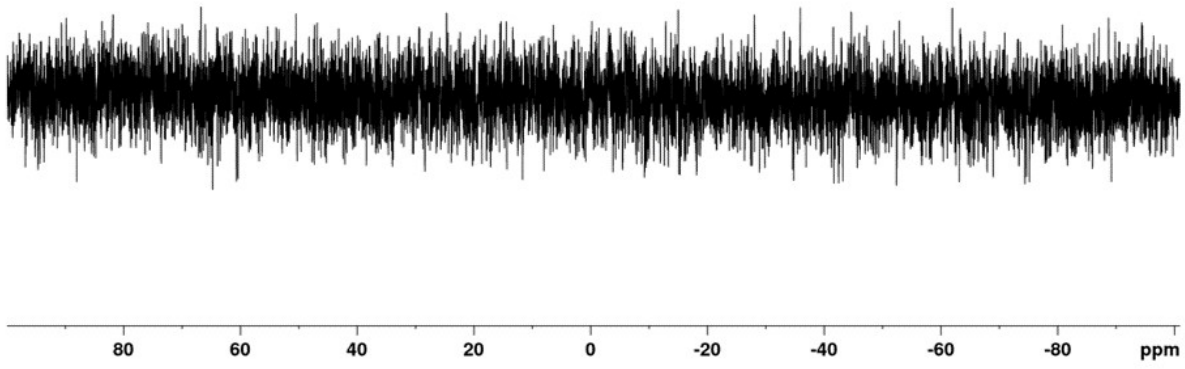


Figure S- 44: ^{7}Li-NMR spectrum (116.66 MHz, 298 K, CD_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the reaction solution after sedimentation.

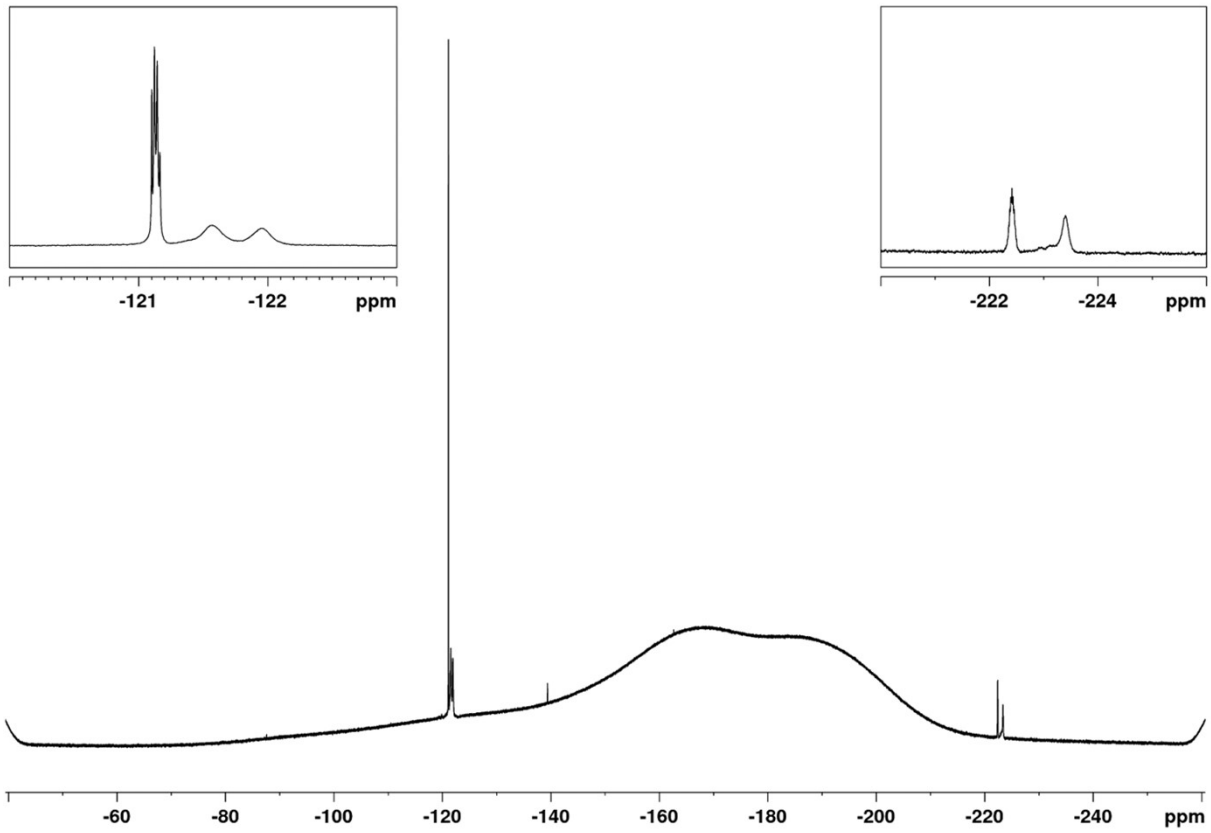


Figure S- 45: ^{19}F-NMR spectrum (282.45 MHz, 298 K, CD_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the reaction solution after sedimentation.

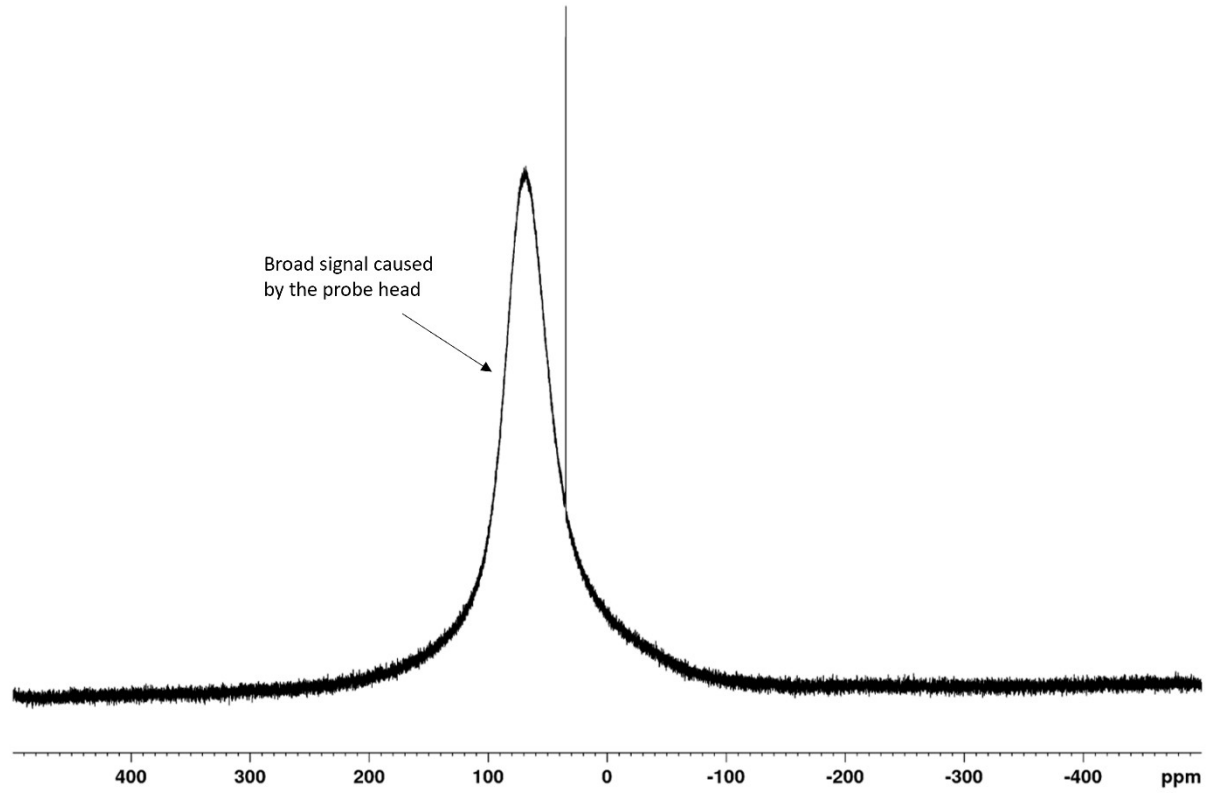


Figure S- 46: ^{7}Li-NMR spectrum (78.22 MHz, 298 K, CD_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the reaction solution after sedimentation.

NMR data of the isolated crystal:

^{1}H-NMR (300.18 MHz, 298 K, CD_2Cl_2): δ = 4.04 (br. s, 1H, $C_{10}F_{15}OH$), 7.20 (m, 2H, *o*-DFB), 7.30 (m, 2H, *o*-DFB), 7.68 (d, *o*-CH, 6H $[Ph_3C][Al(OC_{10}F_{15})_4]$, 7.91 (t, *m*-CH, 6H $[Ph_3C][Al(OC_{10}F_{15})_4]$), 8.30 (t, *p*-CH, 3H $[Ph_3C][Al(OC_{10}F_{15})_4]$) ppm.

^{7}Li-NMR (116.66 MHz, 298 K, CD_2Cl_2): no signal (as expected)

^{19}F-NMR (282.45 MHz, 298 K, CD_2Cl_2): δ = −223.4 (m, C**F**, 12F, $[Ph_3C][Al(OC_{10}F_{15})_4]$), −222.4 (m, C**F**, 3F, $C_{10}F_{15}OH$), −139.4 (m, 2F, *o*-DFB), −121.8 (m, C**F$_2$**, 48F, $[Ph_3C][Al(OC_{10}F_{15})_4]$), −121.1 (m, C**F**, 12F, $C_{10}F_{15}OH$) ppm.

^{27}Al-NMR (78.22 MHz, 298 K, CD_2Cl_2): δ = 34.7 (s, 1Al, $[Ph_3C][$**Al**$(OC_{10}F_{15})_4]$) ppm.

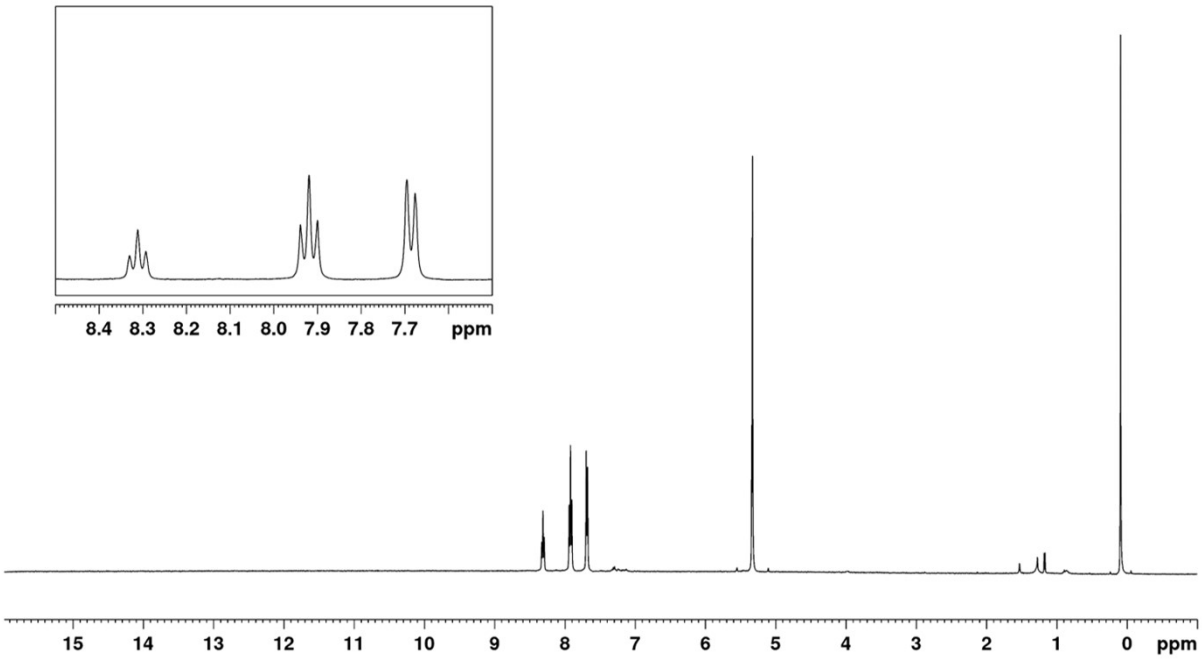


Figure S- 47: ^{1}H-NMR spectrum (400.17 MHz, 298 K, CD_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals.

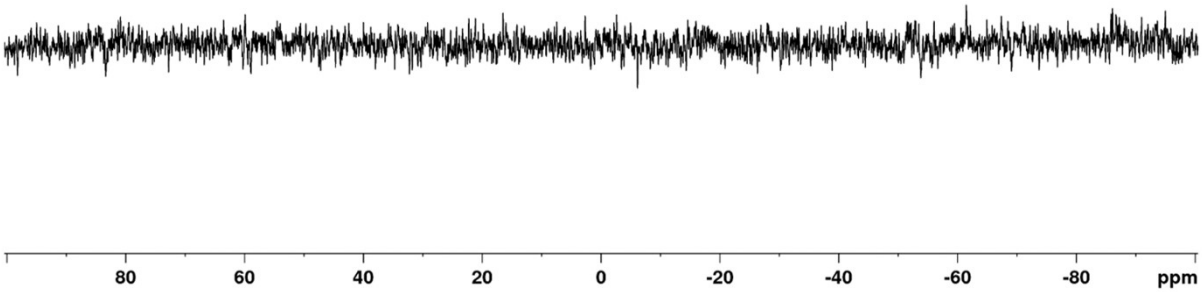


Figure S- 48: ^{7}Li-NMR spectrum (155.52 MHz, 298 K, CD_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals.

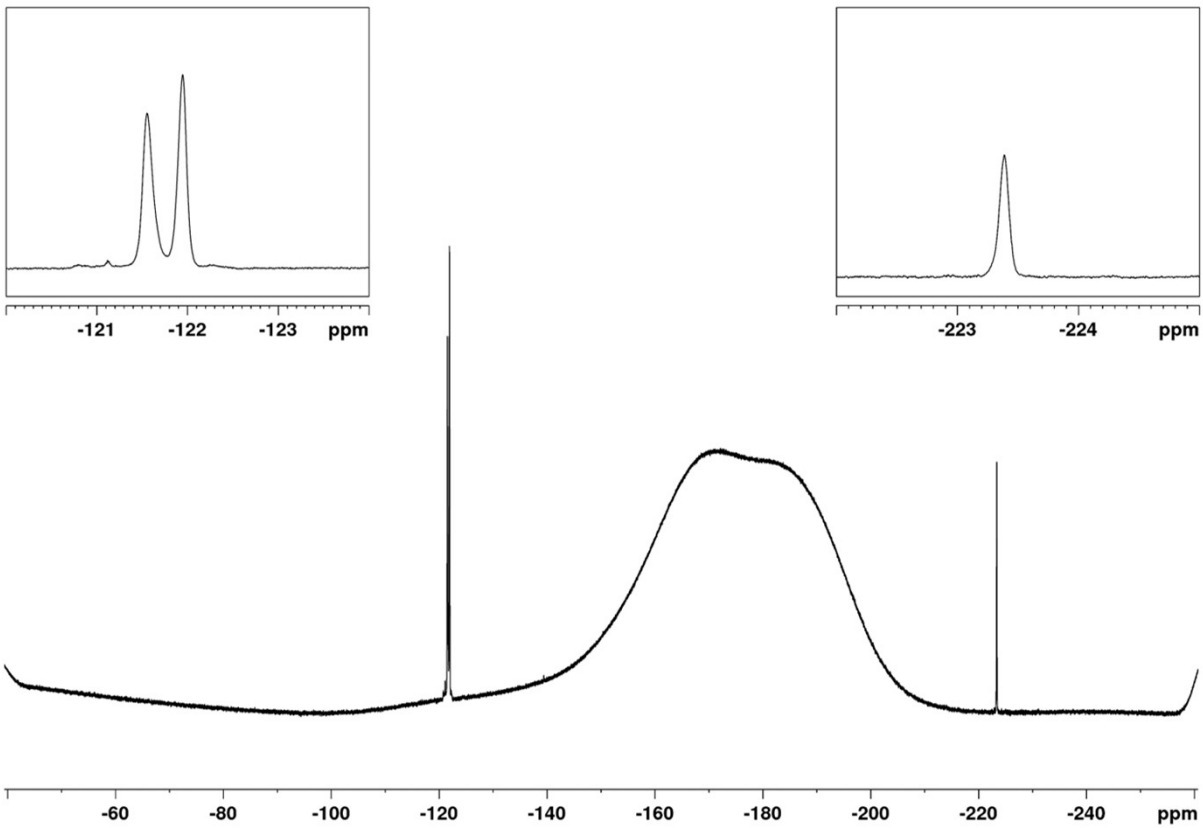


Figure S- 49: ^{19}F-NMR spectrum (376.54 MHz, 298 K, CD_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals.

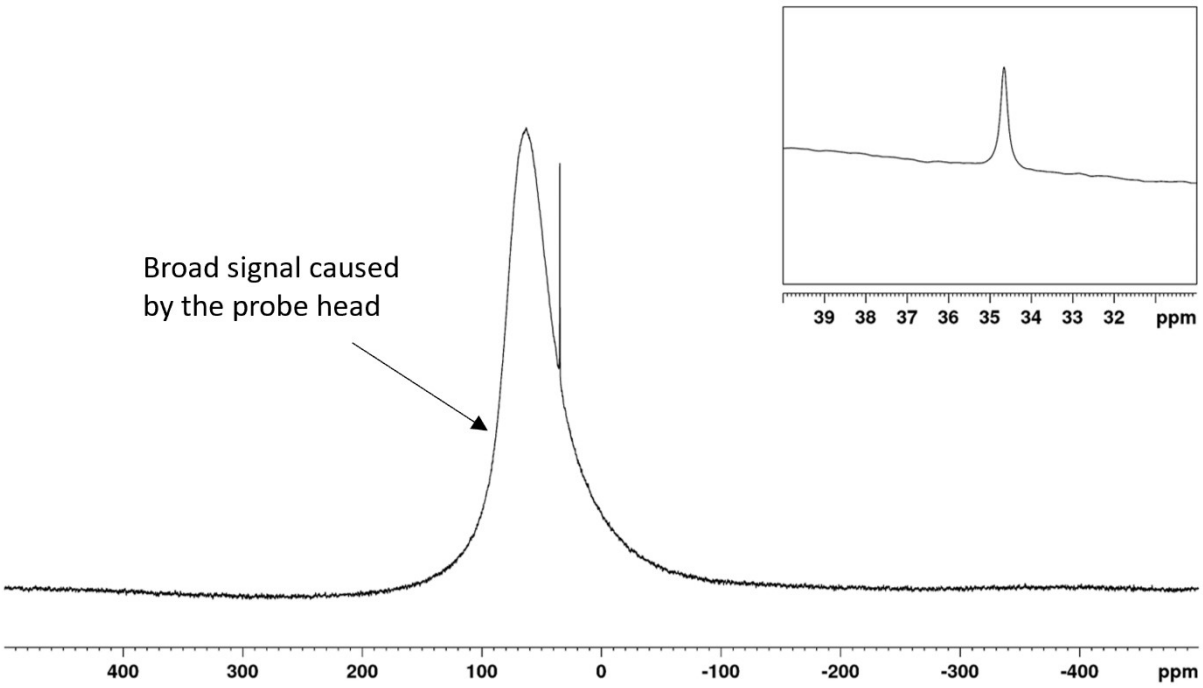


Figure S- 50: ^{27}Al-NMR spectrum (104.27 MHz, 298 K, CD_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals.

Synthesis of $[Ph_3C][Al(OC_{10}F_{15})_4]$

$Li[Al(OC_{10}F_{15})_4]$ (0.260 g, 0.152 mmol) containing impurities of alcohol $C_{10}F_{15}OH$ and Ph_3CCl (0.067 g, 0.240 mmol, 1.59 eq.) were suspended in SO_2 (3.0 mL) and stirred at room temperature for six days. The reaction mixture was allowed to sediment and filtered afterwards. The sedimented solid was extracted five times by condensing SO_2 back, stirring and filtration resulting in an intensive yellow solution on product side and a colorless solid on reactant side. SO_2 was removed under reduced pressure. The yellow solid was washed with CH_2Cl_2 (5.0 mL) in order to remove impurities since the target compound is hardly soluble in CH_2Cl_2 which is illustrated by an NMR of the washing solution and Ph_3CCl was used in excess. The solid residue was dissolved in *o*-DFB (2.0 mL) and crystallized by diffusion crystallization with *n*-pentane (30 mL) for purification (Note: The progress of crystallization could be very well traced by the decolorization of the initially bright yellow solution). The yellow crystals (0.164 g, 0.084 mmol, 55 %; Note: 65% yield considering that the used $Li[Al(OC_{10}F_{15})_4]$ was contaminated by 0.73 eq. of alcohol) were isolated after filtration and characterized by NMR and IR spectroscopy.

NMR data of the washing solution:

^{1}H-NMR (300.18 MHz, 298 K, CD_2Cl_2): δ = 4.29 (br. s, 1H, $C_{10}F_{15}OH$), 7.26 (m, 2H, *o*-DFB), 7.31 (m, 2H, *o*-DFB) ppm.
^{7}Li-NMR (116.66 MHz, 298 K, CD_2Cl_2): δ = −0.7 (br. S, 1Li, Li^+) ppm.
^{19}F-NMR (282.45 MHz, 298 K, CD_2Cl_2): δ = −223.4 (m, C**F**, 12F, Li/$[Ph_3C][Al(OC_{10}F_{15})_4]$), −222.4 (m, C**F**, 3F, $C_{10}F_{15}OH$), −121.8 (m, C**F$_2$**, 48F, $[Ph_3C][Al(OC_{10}F_{15})_4]$), −121.1 (m, C**F**, 12F, $C_{10}F_{15}OH$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, CD_2Cl_2): δ = 34.7 (s, 1Al, Li/$[Ph_3C][$**Al**$(OC_{10}F_{15})_4]$) ppm.

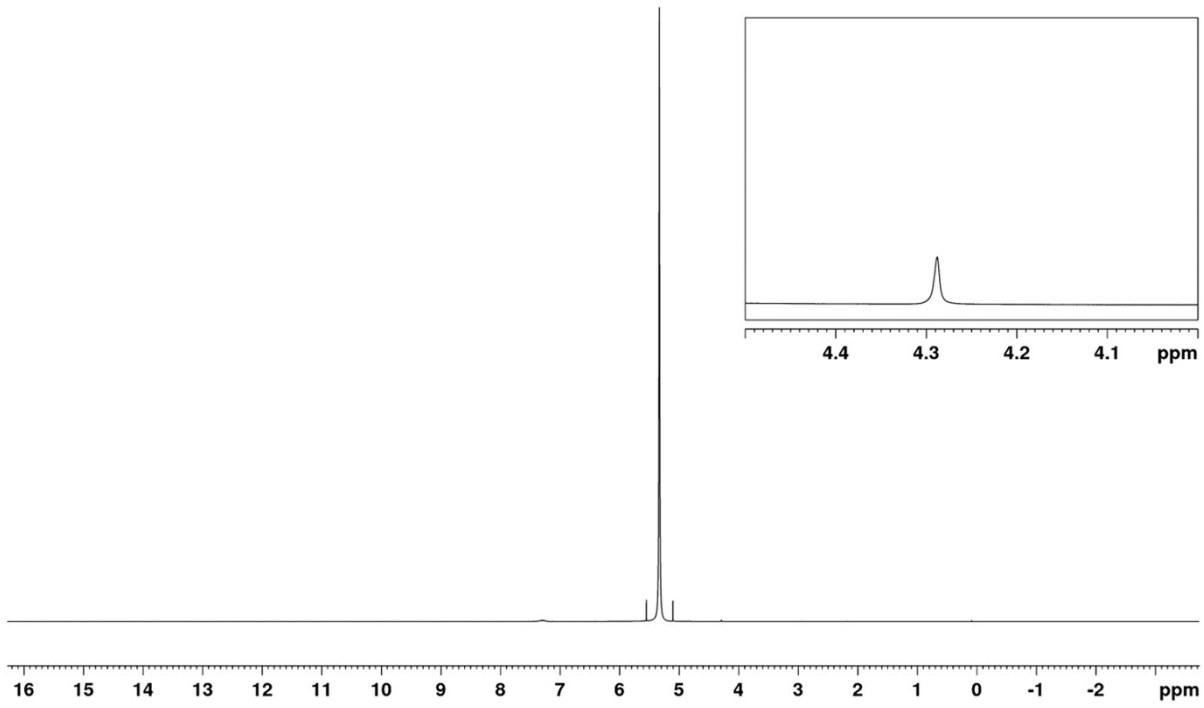


Figure S- 51: ^{1}H-NMR spectrum (400.17 MHz, 298 K, CH_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the washing solution.

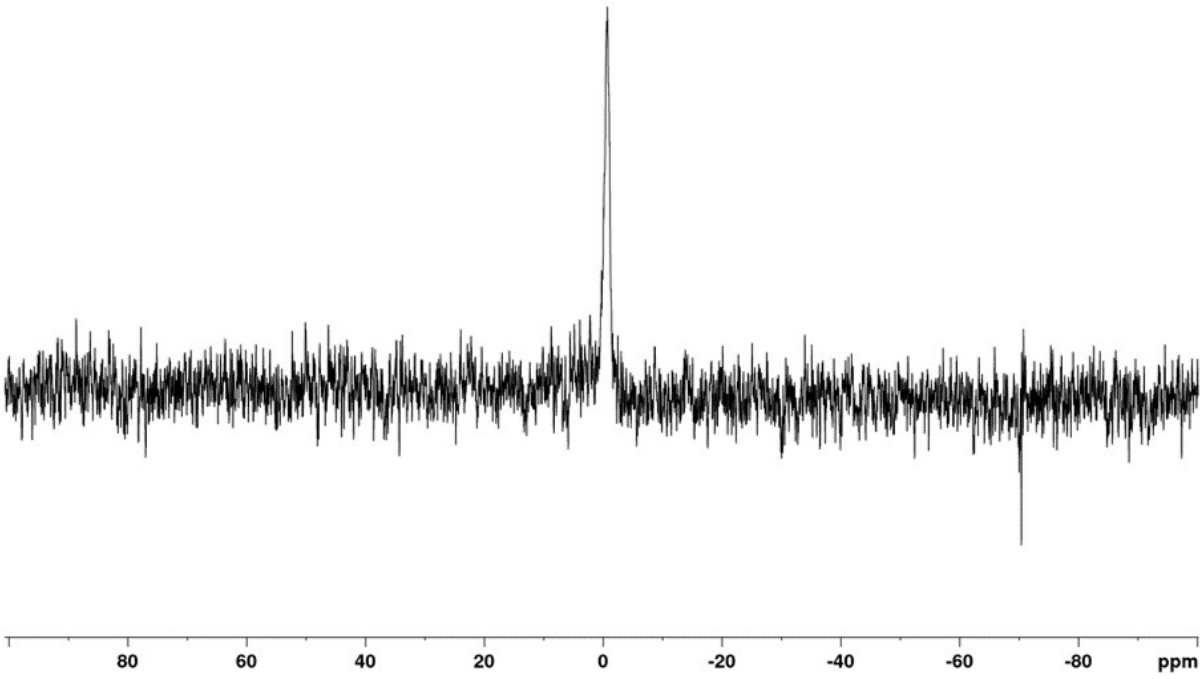


Figure S- 52: ^{7}Li-NMR spectrum (155.52 MHz, 298 K, CH_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the washing solution.

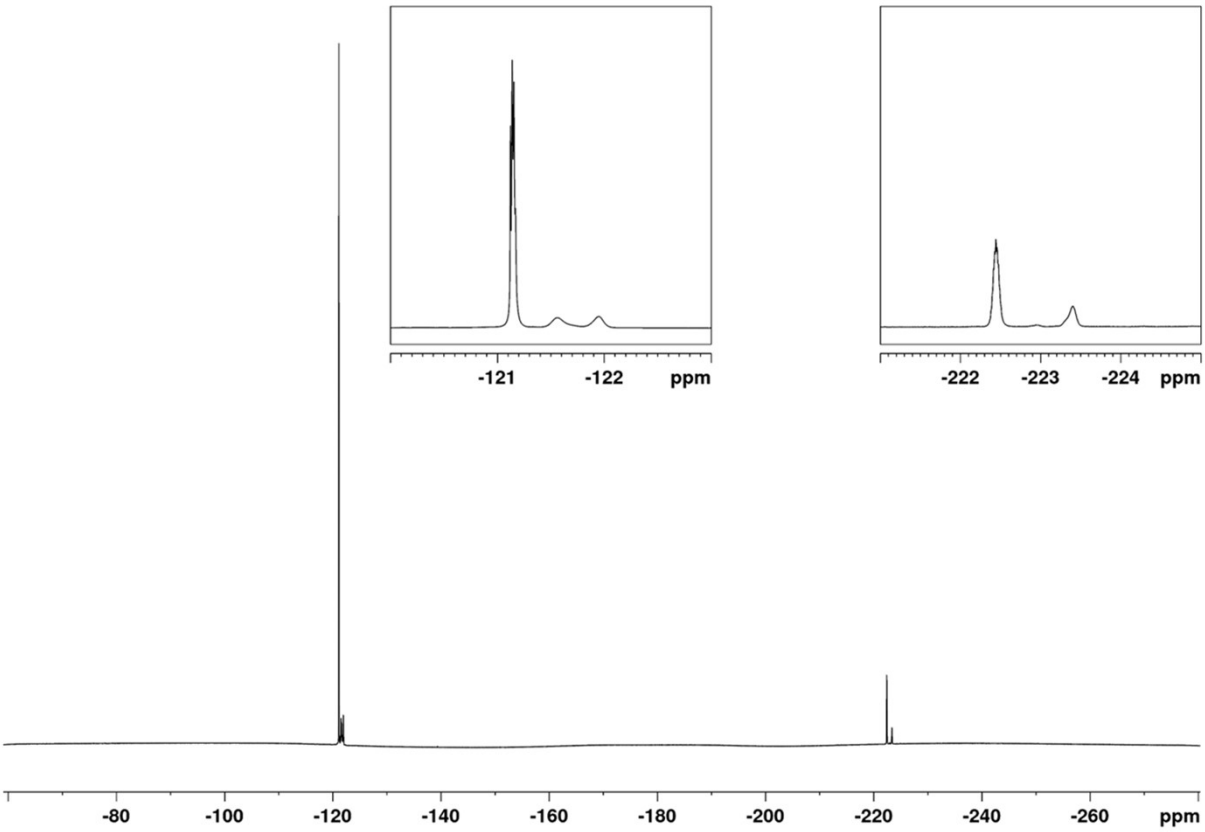


Figure S- 53: ^{19}F-NMR spectrum (376.54 MHz, 298 K, CH_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the washing solution.

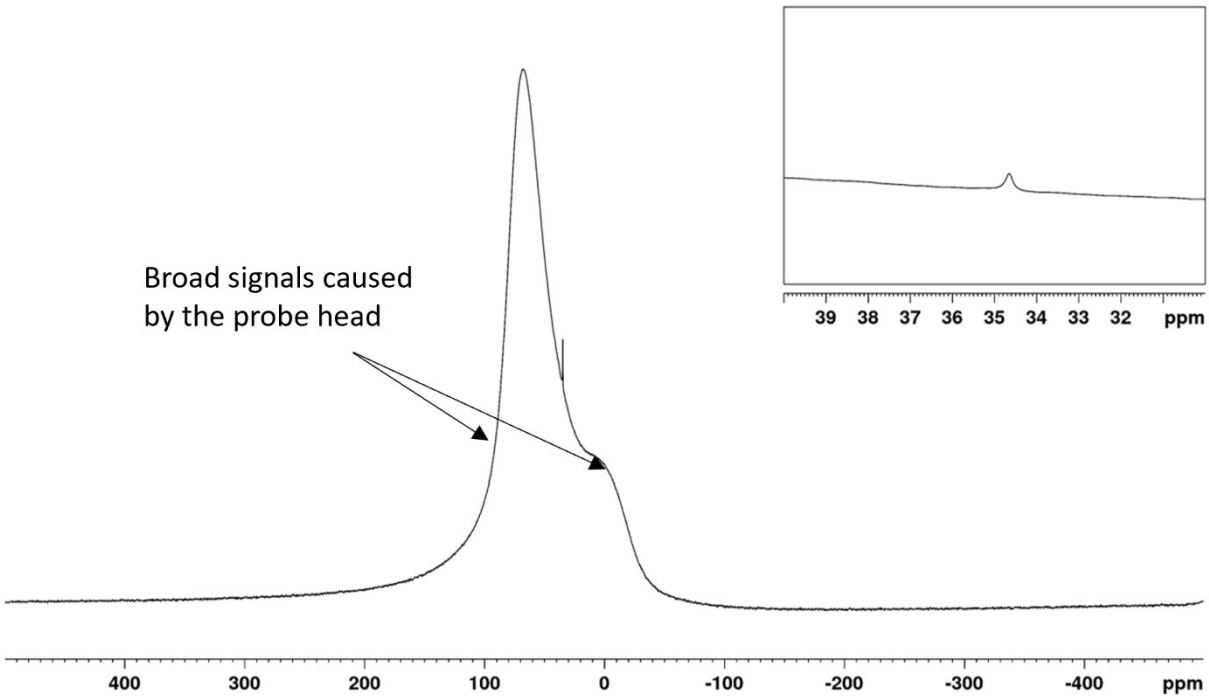


Figure S- 54: ^{27}Al-NMR spectrum (104.27 MHz, 298 K, CH_2Cl_2) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the washing solution.

NMR and IR data of the isolated crystals:

^{1}H-NMR (200.13 MHz, 298 K, CD_3CN): δ = 7.76 (d, *o*-CH, 6H, $[Ph_3C]^+$), 7.92 (t, *m*-CH, 6H, $[Ph_3C]^+$), 8.33 (t, *p*-CH, 3H, $[Ph_3C]^+$) ppm.

^{7}Li-NMR (116.66 MHz, 298 K, CD_3CN): δ = −2.7 (br. S, 1Li, Li^+, **only traces**) ppm.

^{13}C-NMR (50.32 MHz, 298 K, CD_3CN): δ = 130.2 (s, Ph, $[\mathbf{Ph_3}C][Al(OC_{10}F_{15})_4]$, 140.2 (s, Ph, $[\mathbf{Ph_3}C][Al(OC_{10}F_{15})_4]$, 143.1 (s, Ph, $[\mathbf{Ph_3}C][Al(OC_{10}F_{15})_4]$, 143.2 (s, Ph, $[\mathbf{Ph_3}C][Al(OC_{10}F_{15})_4]$, 212.1 (s, $Ph_3\mathbf{C}^+$, $[Ph_3\mathbf{C}][Al(OC_{10}F_{15})_4]$ ppm.

^{19}F-NMR (282.45 MHz, 298 K, CD_3CN): δ = −223.7 (m, C**F**, 12F, $[Ph_3C][Al(OC_{10}F_{15})_4]$), −122.0 (m, C$\mathbf{F_2}$, 48F, $[Ph_3C][Al(OC_{10}F_{15})_4]$) ppm.

^{27}Al-NMR (78.22 MHz, 298 K, CD_3CN): δ = 34.8 (s, 1Al, $[Ph_3C][\mathbf{Al}(OC_{10}F_{15})_4]$) ppm.

FTIR (Diamant, ATR): $\tilde{\nu}$ = 1585 (w), 1486 (vw), 1454 (vw), 1360 (w), 1293 (w), 1269 (vs), 1189 (vw), 1105 (vw), 978 (m), 955 (vs), 843 (vw), 807 (vw), 767 (vw), 756 (vw), 704 (vw), 678 (vw), 650 (vw), 624 (vw), 609 (vw), 533 (vw), 467 (vw), 441 (vw), 402 (vw) cm^{-1}.

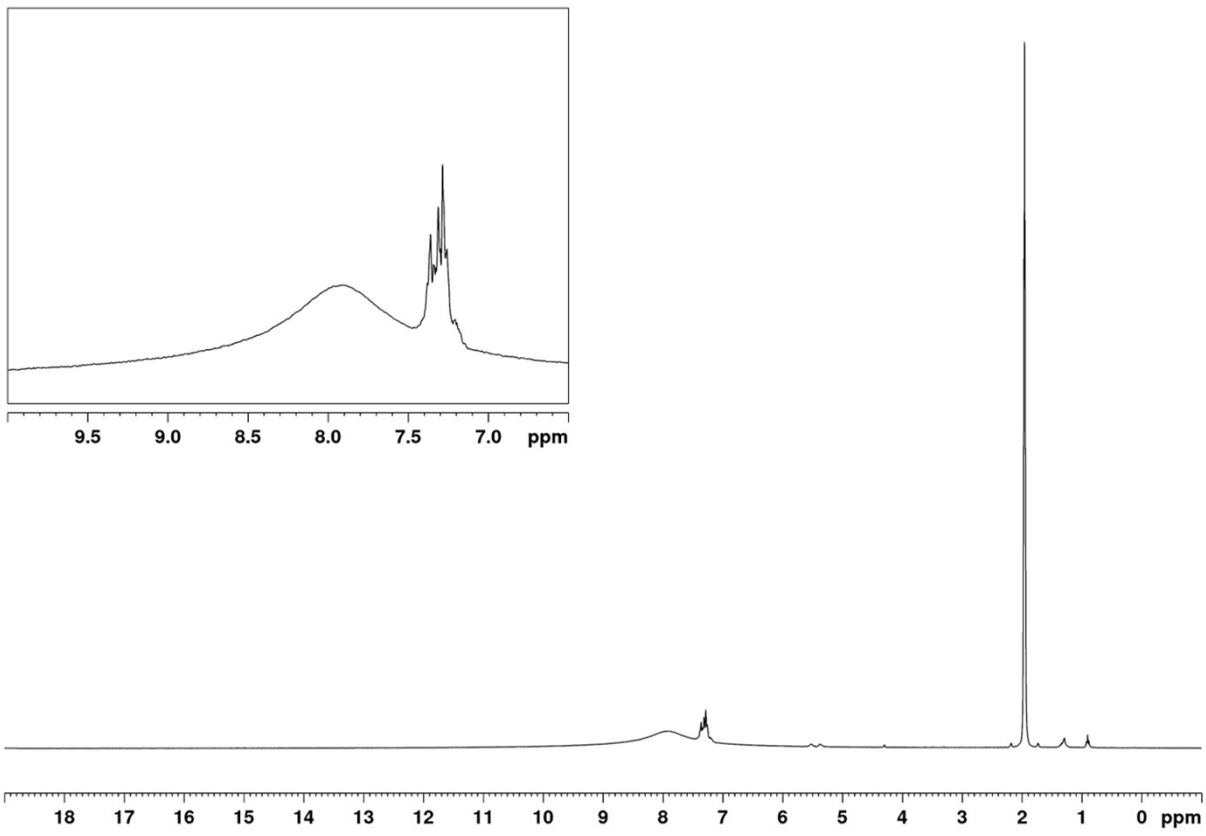


Figure S- 55: ^{1}H-NMR spectrum (300.18 MHz, 298 K, CD_3CN) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals.

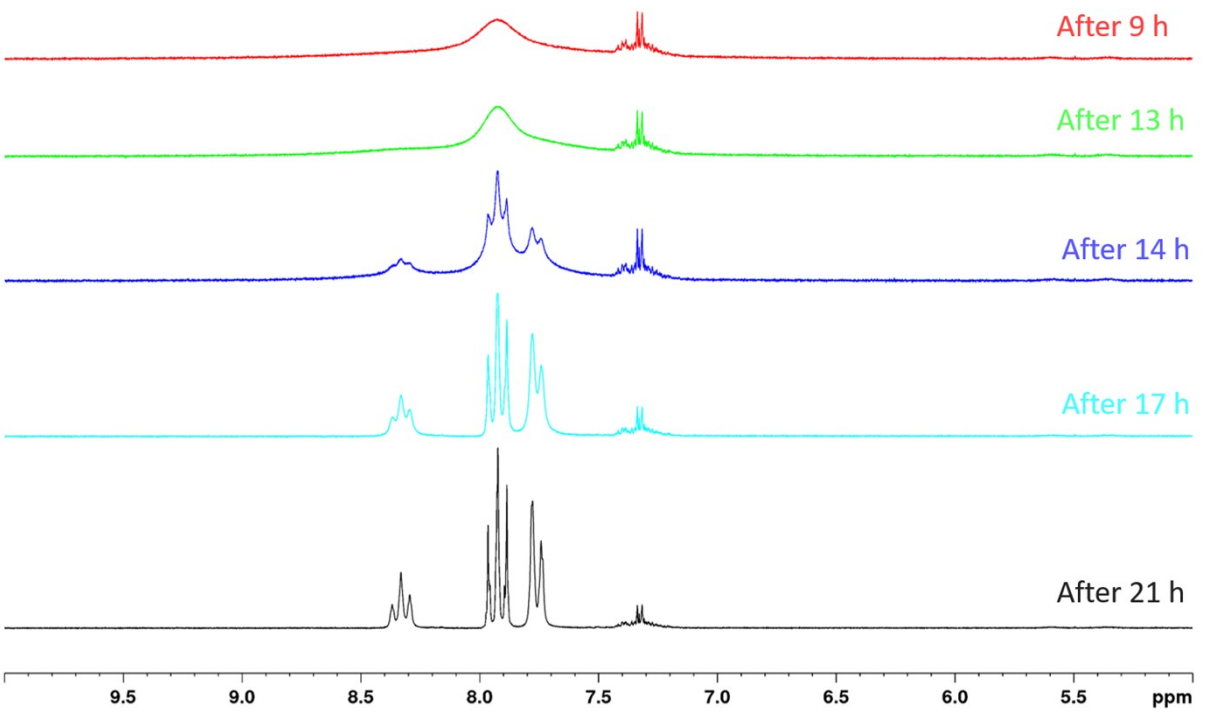


Figure S- 56: ^{1}H-NMR spectra (200.13 MHz, 298 K, CD_3CN) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals measured at different times after sample preparation.

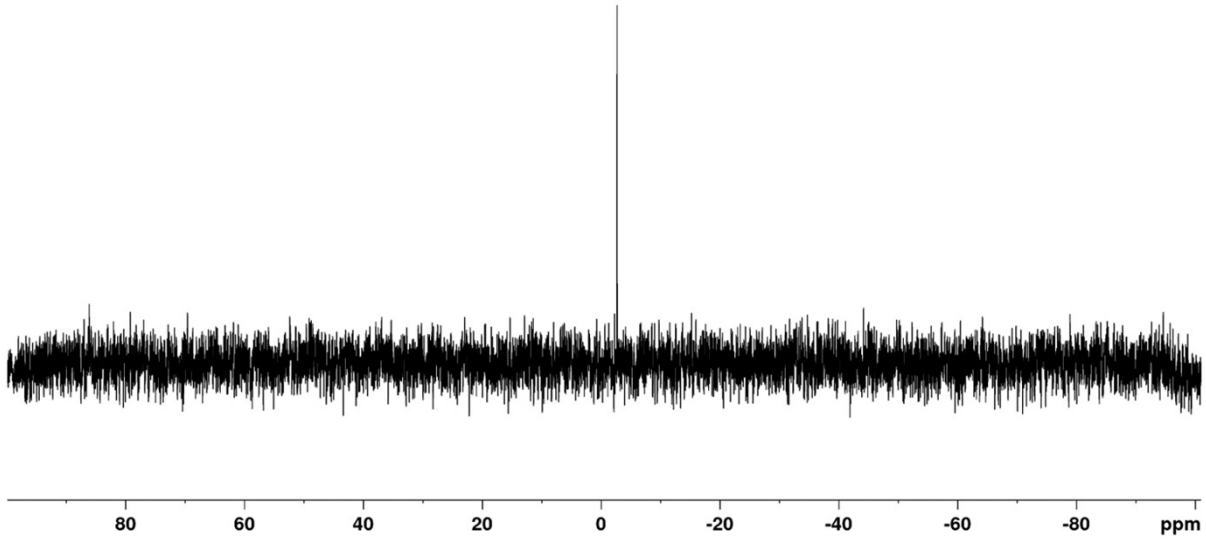


Figure S- 57: ^{7}Li-NMR spectrum (116.66 MHz, 298 K, CD_3CN) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals => only traces of Li^+.

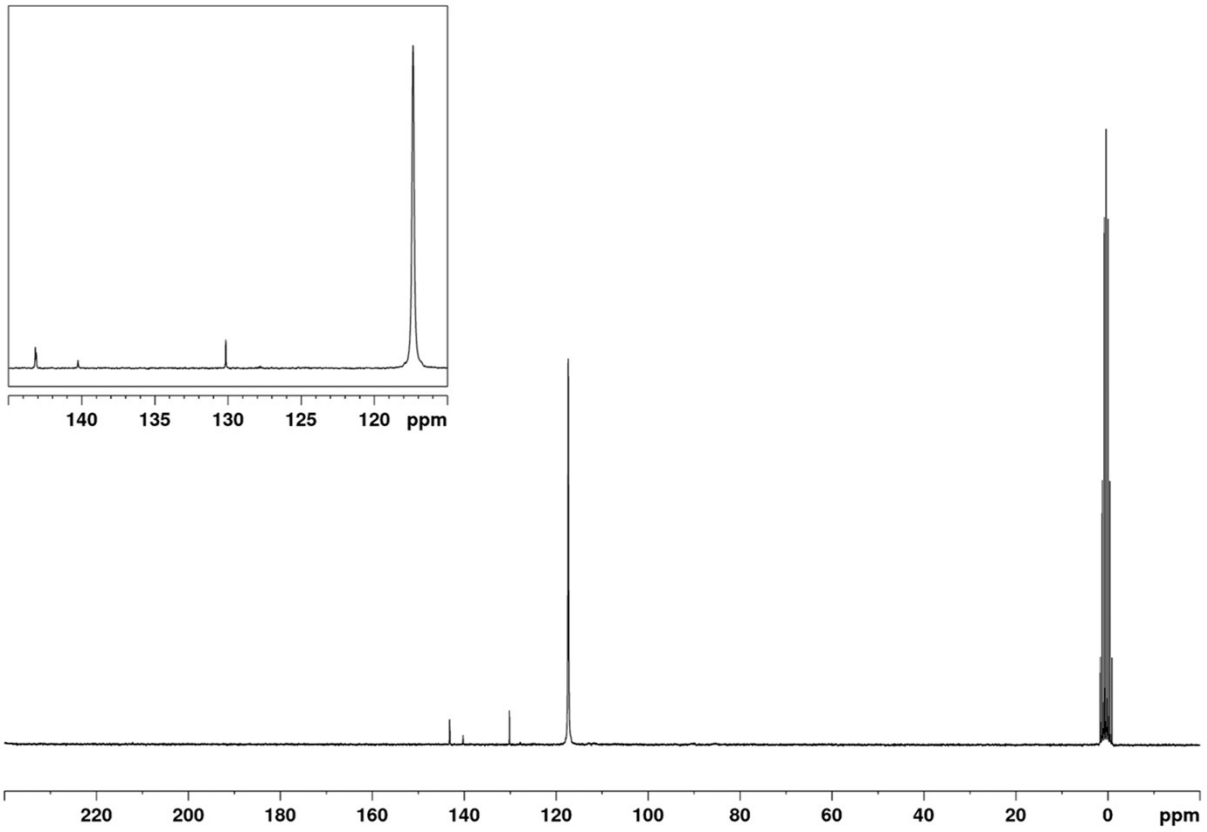


Figure S- 58: ^{13}C-NMR spectrum (50.32 MHz, 298 K, CD_3CN) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals.

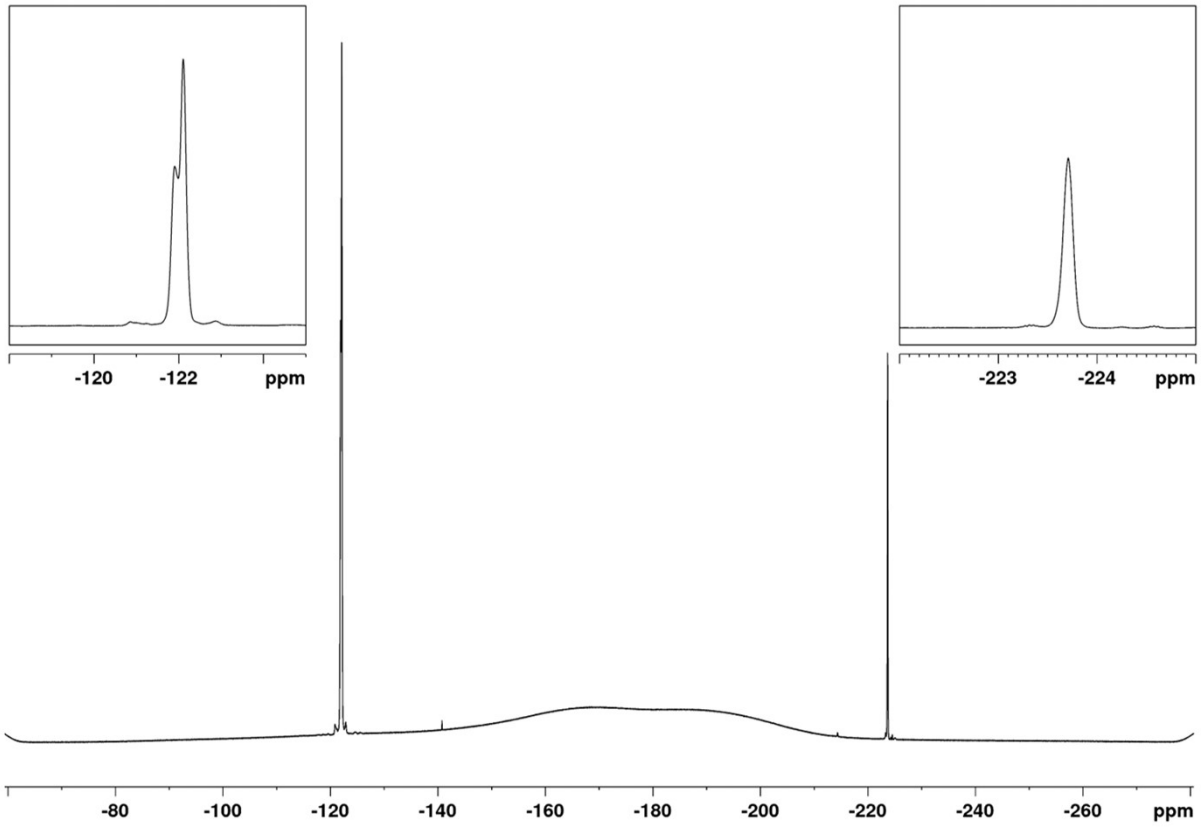


Figure S- 59: ^{19}F-NMR spectrum (282.45 MHz, 298 K, CD_3CN) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals.

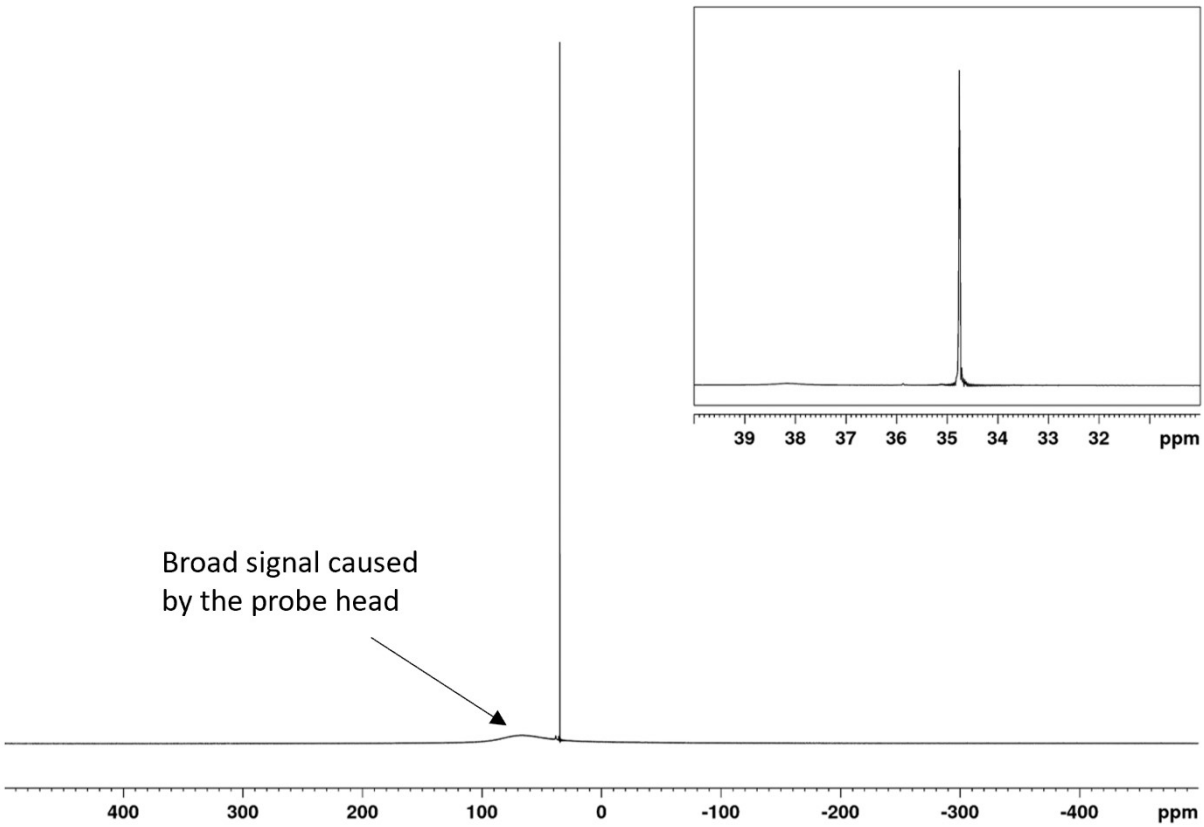


Figure S- 60: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, CD_3CN) of $[Ph_3C][Al(OC_{10}F_{15})_4]$ of the isolated crystals.

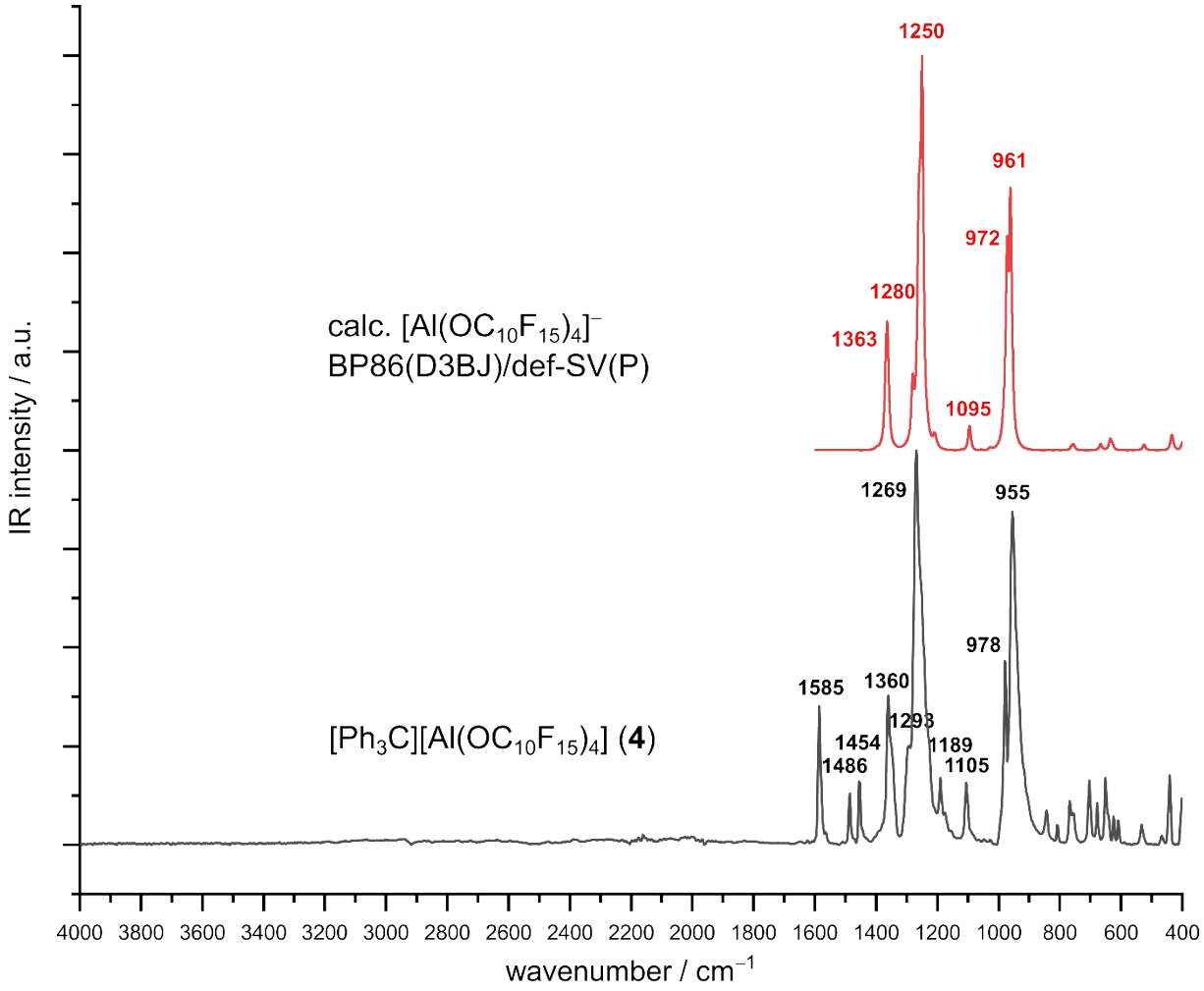


Figure S- 61: IR spectrum of $[Ph_3C][Al(OC_{10}F_{15})_4]$ (black) in comparison with the calculated IR spectrum of the $[pfAd]^-$ anion at BP86(D3BJ)/def-SV(P) level of theory (red). All IR data of obtained pure substances of the $[pfAd]^-$ anion are compared and assigned in Table S- 1.

Synthesis of $[NO][Al(OC_{10}F_{15})_4]$ containing impurities of $C_{10}F_{15}OH$

$Li[Al(OC_{10}F_{15})_4]$ (0.304 g, 0.177 mmol) containing impurities of alcohol $C_{10}F_{15}OH$ and $[NO][BF_4]$ (0.025 g, 0.214 mmol, 1.21 eq.) were suspended in SO_2 (3.0 mL) and stirred for 4 d at r.t. The reaction mixture was allowed to sediment and filtered. The solid residue was extracted once by condensing SO_2 back followed by filtration. SO_2 was removed under reduced pressure and the orange solid residue was washed with C_6F_6 (2.5 mL). The solvent was removed and the solid residue dried under reduced pressure and the target compound obtained as orange solid (0.143 g, 0.082 mmol, 46 %) containing impurities of alcohol.

^{1}H-NMR (400.17 MHz, 298 K, *o*-DFB): δ = 4.09 (m, 1H, $C_{10}F_{15}$O**H**) ppm.

^{7}Li-NMR (155.52 MHz, 298 K, *o*-DFB): no signal (as expected)

^{14}N-NMR (28.91 MHz, 298 K, *o*-DFB): δ = 265.5 (N_2) ppm.

^{19}F-NMR (376.54 MHz, 298 K, *o*-DFB): δ = −223.2 (m, C**F**, 12F, $[NO][Al(OC_{10}F_{15})_4]$), −222.8 (m, C**F**, 3F, $C_{10}F_{15}OH$), −163.6 (m, 6F, C_6F_6), −121.5 (m, C**F$_2$**, 12F, $C_{10}F_{15}OH$), −121.3 (m, C**F$_2$**, 48F, $[NO][Al(OC_{10}F_{15})_4]$) ppm.

^{27}Al-NMR (104.27 MHz, 298 K, *o*-DFB): δ = 35.4 (s, 1Al, $[NO][$**Al**$(OC_{10}F_{15})_4]$) ppm.

FT-Raman: $\tilde{\nu}$ = 2332 (vw), 1292 (m), 1148 (vw), 727 (vw), 700 (vw), 667 (vw), 630 (vw), 573 (w), 500 (vw), 442 (w), 403 (vs), 372 (vs), 311 (s) cm^{-1}.

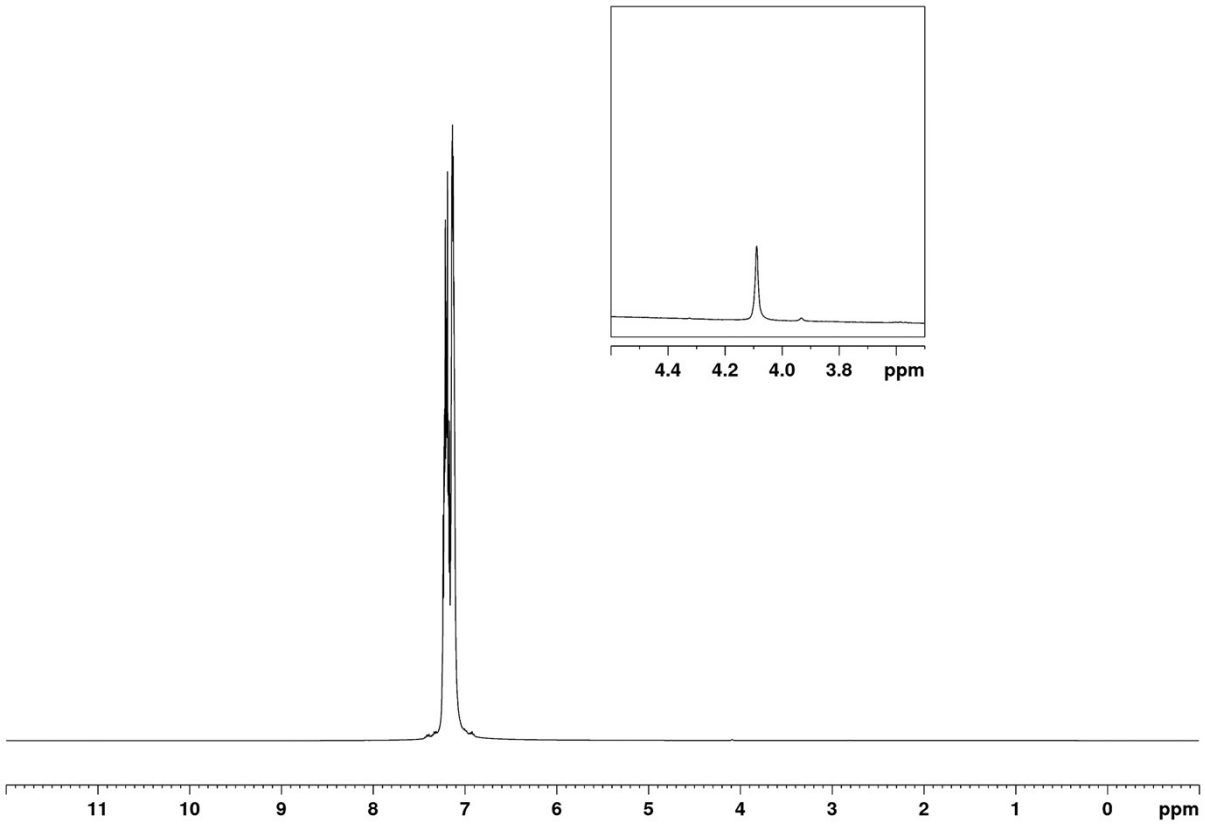


Figure S- 62: ^{1}H-NMR (400.17 MHz, 298 K, *o*-DFB) Synthesis of [NO][Al($OC_{10}F_{15}$)$_4$] containing impurities of $C_{10}F_{15}OH$.

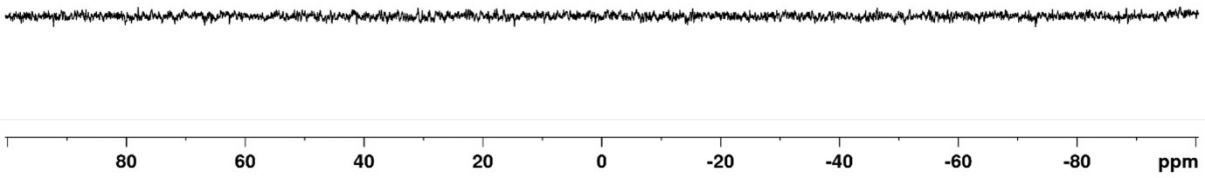


Figure S- 63: ^{7}Li-NMR (155.52 MHz, 298 K, *o*-DFB) Synthesis of [NO][Al($OC_{10}F_{15}$)$_4$] containing impurities of $C_{10}F_{15}OH$.

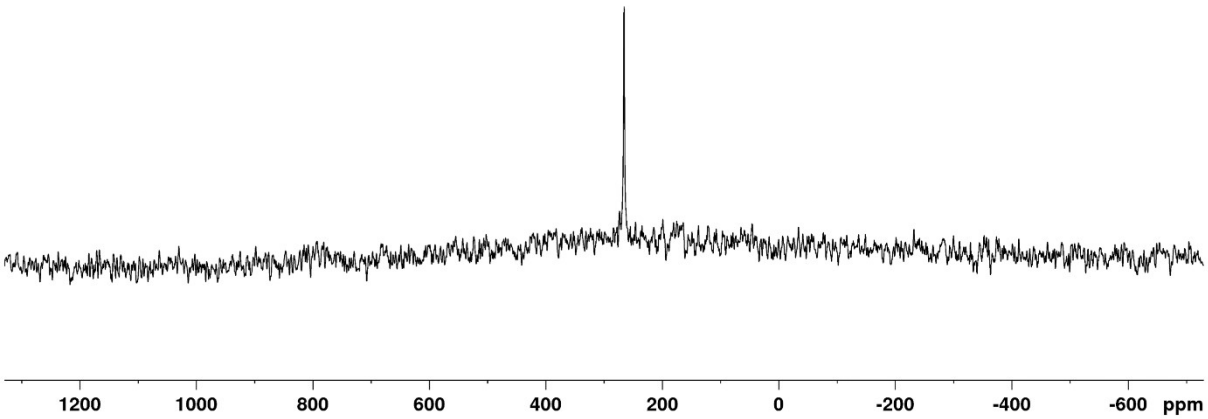


Figure S- 64: ^{14}N-NMR (28.91 MHz, 298 K, *o*-DFB) Synthesis of [NO][Al($OC_{10}F_{15}$)$_4$] containing impurities of $C_{10}F_{15}OH$.

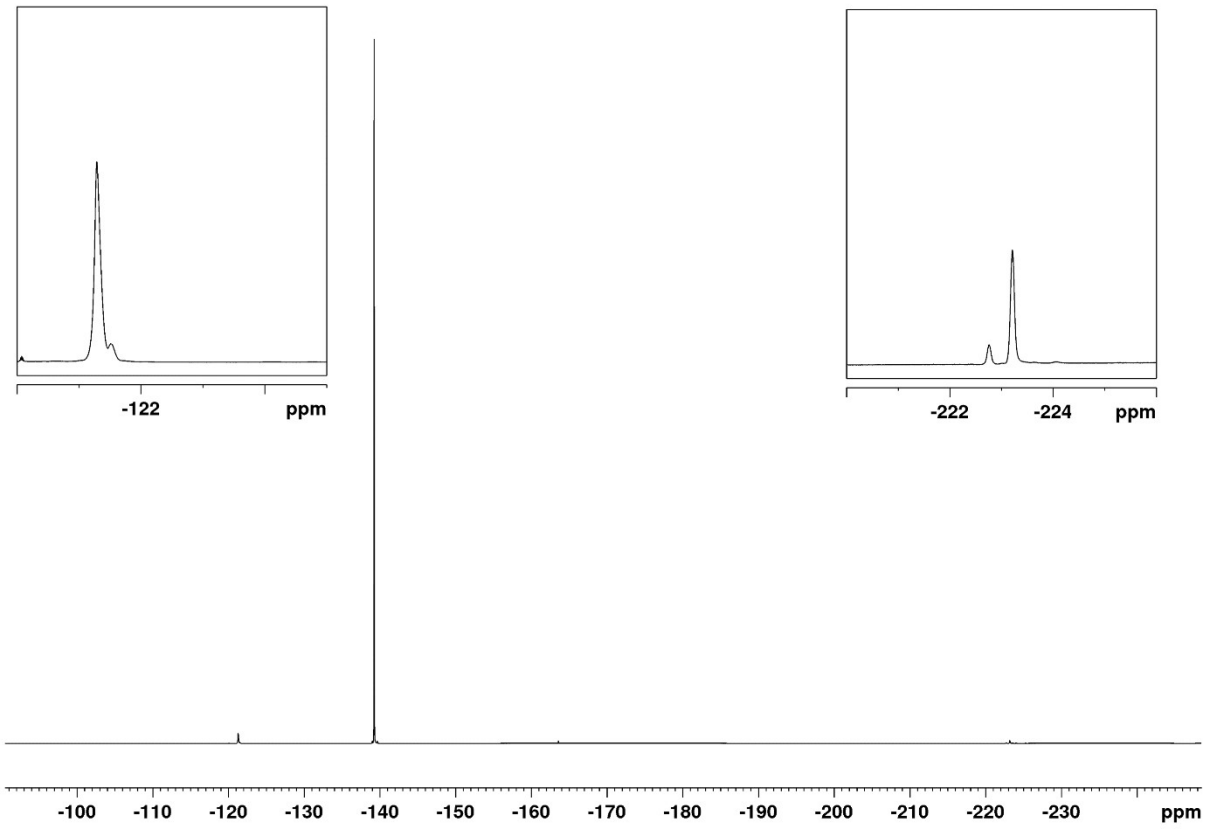


Figure S- 65: ^{19}F-NMR (376.54 MHz, 298 K, *o*-DFB) Synthesis of [NO][Al(OC$_{10}$F$_{15}$)$_4$] containing impurities of C$_{10}$F$_{15}$OH.

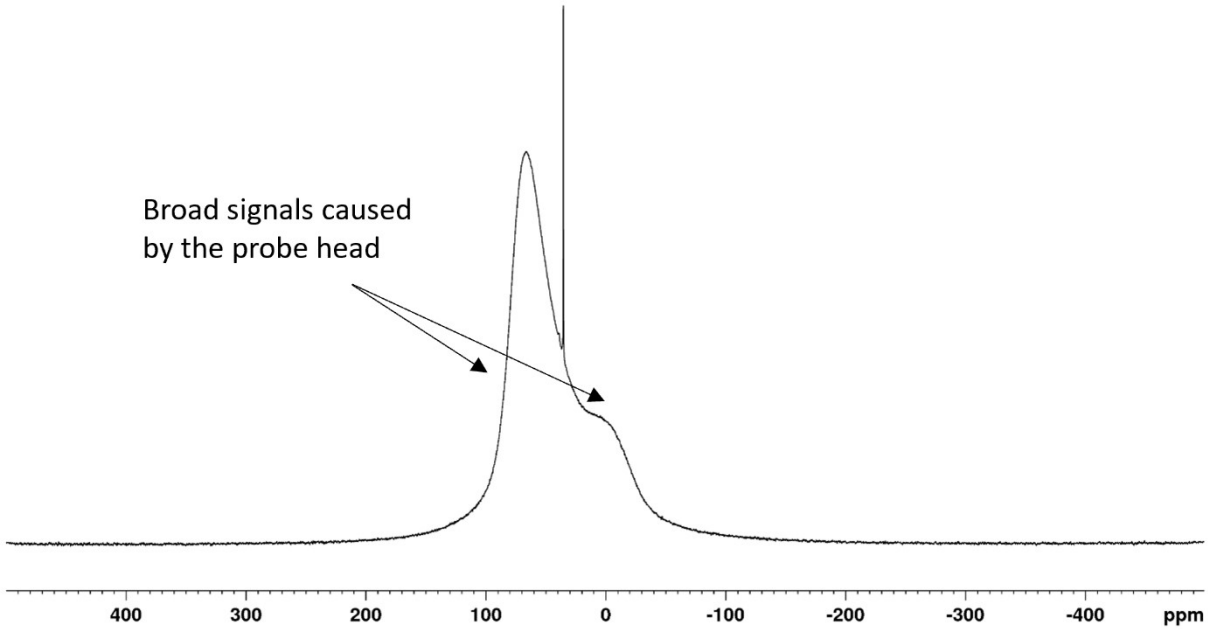
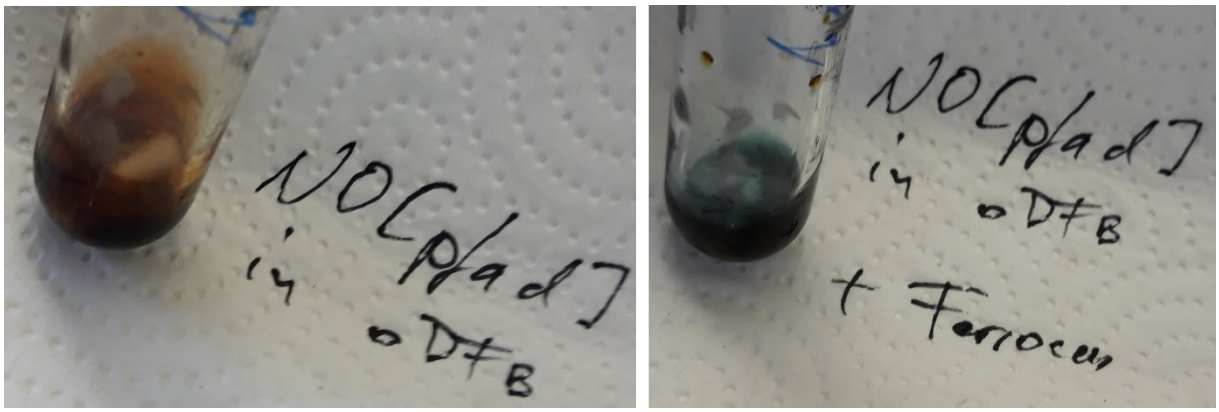


Figure S- 66: ^{27}Al-NMR (104.27 MHz, 298 K, *o*-DFB) Synthesis of [NO][Al(OC$_{10}$F$_{15}$)$_4$] containing impurities of C$_{10}$F$_{15}$OH.

Since Crystallization of [NO][Al(OC$_{10}$F$_{15}$)$_4$] was not successful as well as the Raman spectrum does not show a clear vibration band indicating the presence of NO^+ the property as potential oxidizing agent what would be expected for NO^+ was visualized by addition of a small amount of ferrocene to a solution of [NO][Al(OC$_{10}$F$_{15}$)$_4$] in *o*-DFB. After addition the color changed from orange/brown to blue.



The absence of Li^+ and the observations described above (anion is present) allow the conclusion that the synthesis of $[NO][Al(OC_{10}F_{15})_4]$ was successful, albeit with an impurity of the alcohol $C_{10}F_{15}OH$.

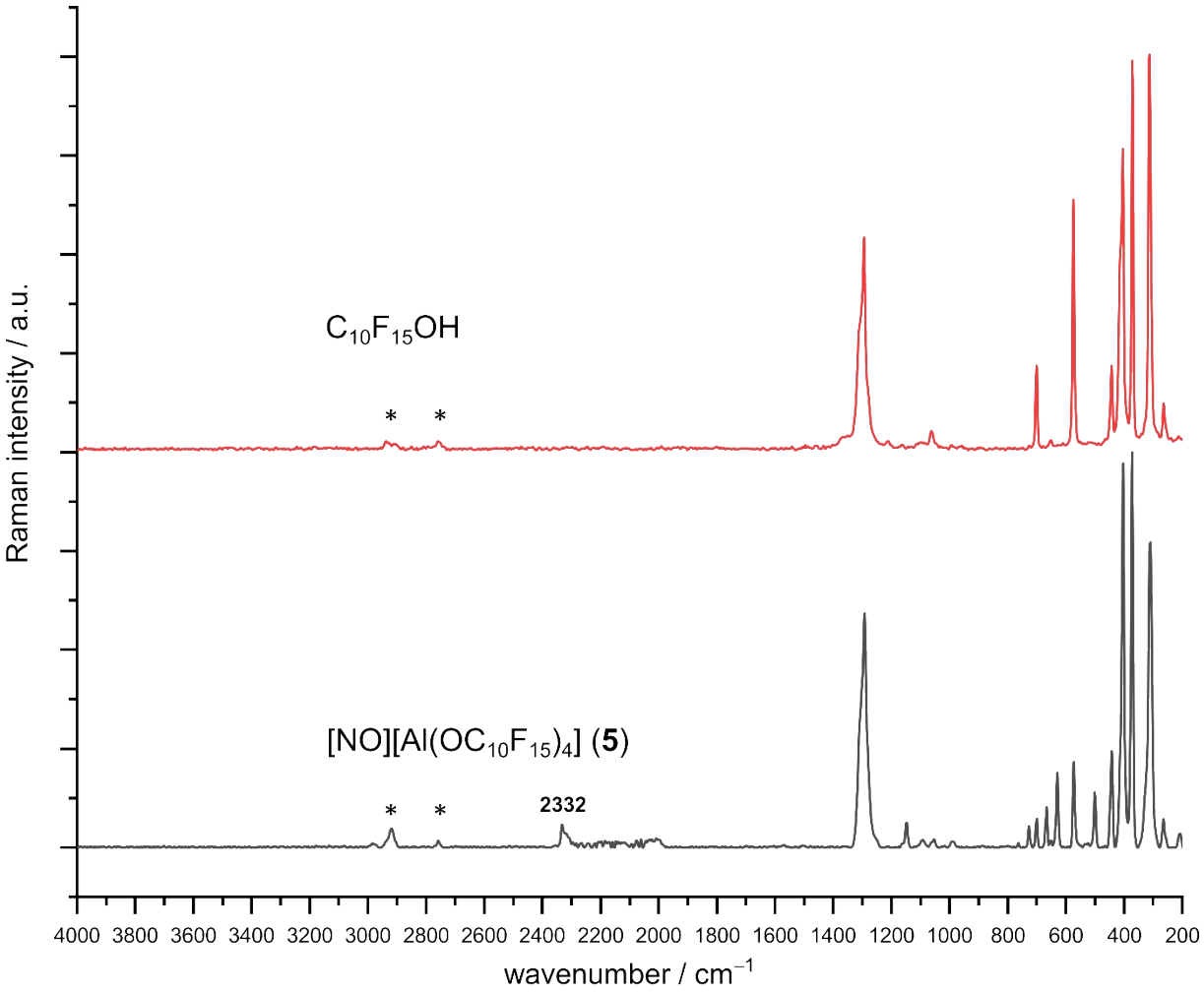


Figure S- 67: Raman spectrum (1000 scans, 100 mW) of $[NO][Al(OC_{10}F_{15})_4]$ (black) and $C_{10}F_{15}OH$ (red). The bands marked with "*" are artifacts of the spectrometer.

Synthesis of $[P_9][Al(OC_{10}F_{15})_4]$ containing impurities of $C_{10}F_{15}OH$

$[NO][Al(OC_{10}F_{15})_4]$ (0.060 g, 0.034 mmol, containing impurities of alcohol $C_{10}F_{15}OH$) and P_4 (0.011 g, 0.089 mmol, 2.60 eq) were submitted into a *J. Young* valve NMR tube. After addition of CH_2Cl_2 (0.5 mL) the reaction mixture was sonicated for 20 h. A yellow solution containing also undissolved solid was

obtained and analyzed by NMR spectroscopy.

NMR data of the NMR valve reaction in CH_2Cl_2:

^{1}H-NMR (200.13 MHz, 298 K, CH_2Cl_2): δ = 3.94 (br. s, 1H, $C_{10}F_{15}OH$) ppm.
^{19}F-NMR (188.31 MHz, 298 K, CH_2Cl_2): δ = −223.6 (m, C**F**, 12F, $[P_9][Al(OC_{10}F_{15})_4]$), −222.5 (m, C**F**, 3F, $C_{10}F_{15}OH$), −121.9 (m, C**F_2**, $[P_9][Al(OC_{10}F_{15})_4]$), −121.5 (m, C**$F_2$**, $[P_9][Al(OC_{10}F_{15})_4]$), −121.1 (m, C**$F_2$**, 12F, $C_{10}F_{15}OH$) ppm.
^{31}P-NMR (81.01 MHz, 298 K, CH_2Cl_2): δ = −522.1 (s, 4P, P_4), −247.3 (m, 4P, $[P_9]^+$, P_C, $[\mathbf{P_2}P_2PP_2'\mathbf{P_2'}]^+$), 61.4 (m, 1P, $[P_9]^+$, P_B, $[P_2P_2\mathbf{P}PP_2'P_2']^+$), 110.5 (m, 4P, $[P_9]^+$, P_A, $[P_2\mathbf{P_2}P\mathbf{P_2'}P_2']^+$) ppm.

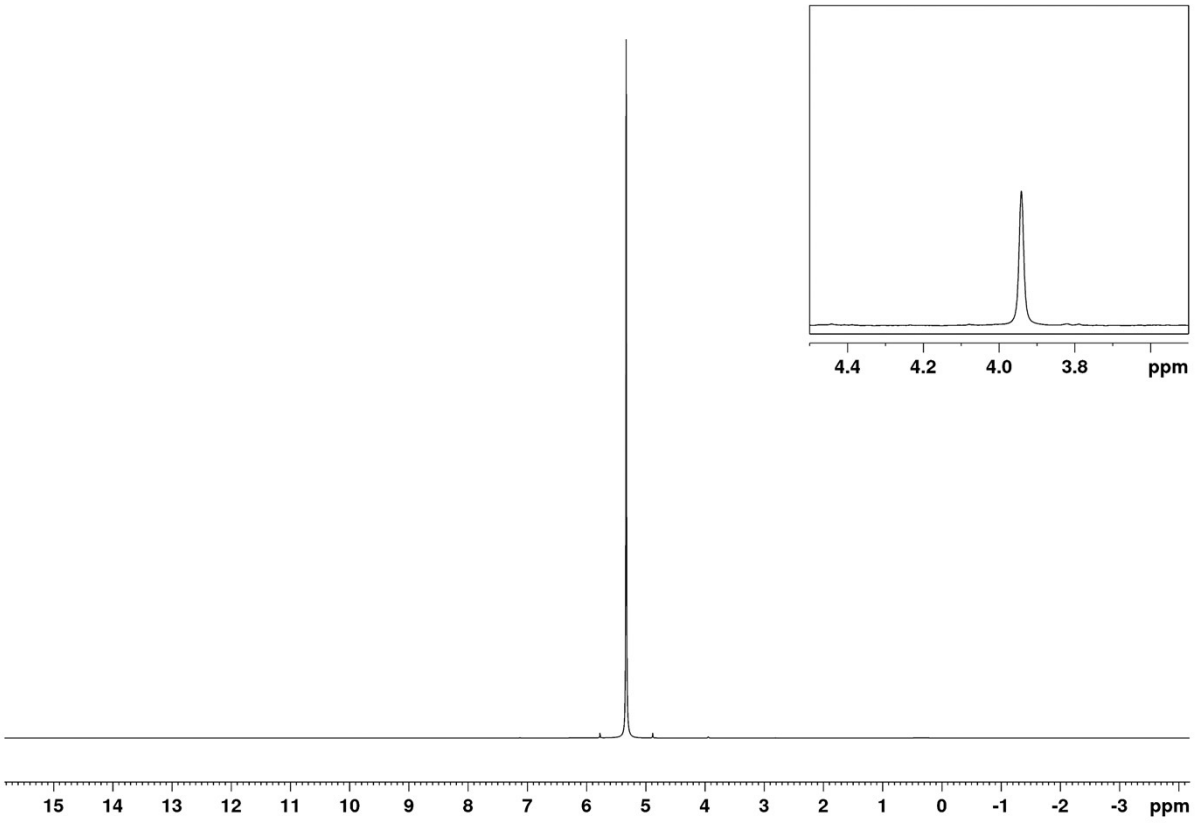


Figure S- 68: ^{1}H-NMR (200.13 MHz, 298 K, CH_2Cl_2) of $[NO][Al(OC_{10}F_{15})_4]$ and P_4 in CH_2Cl_2.

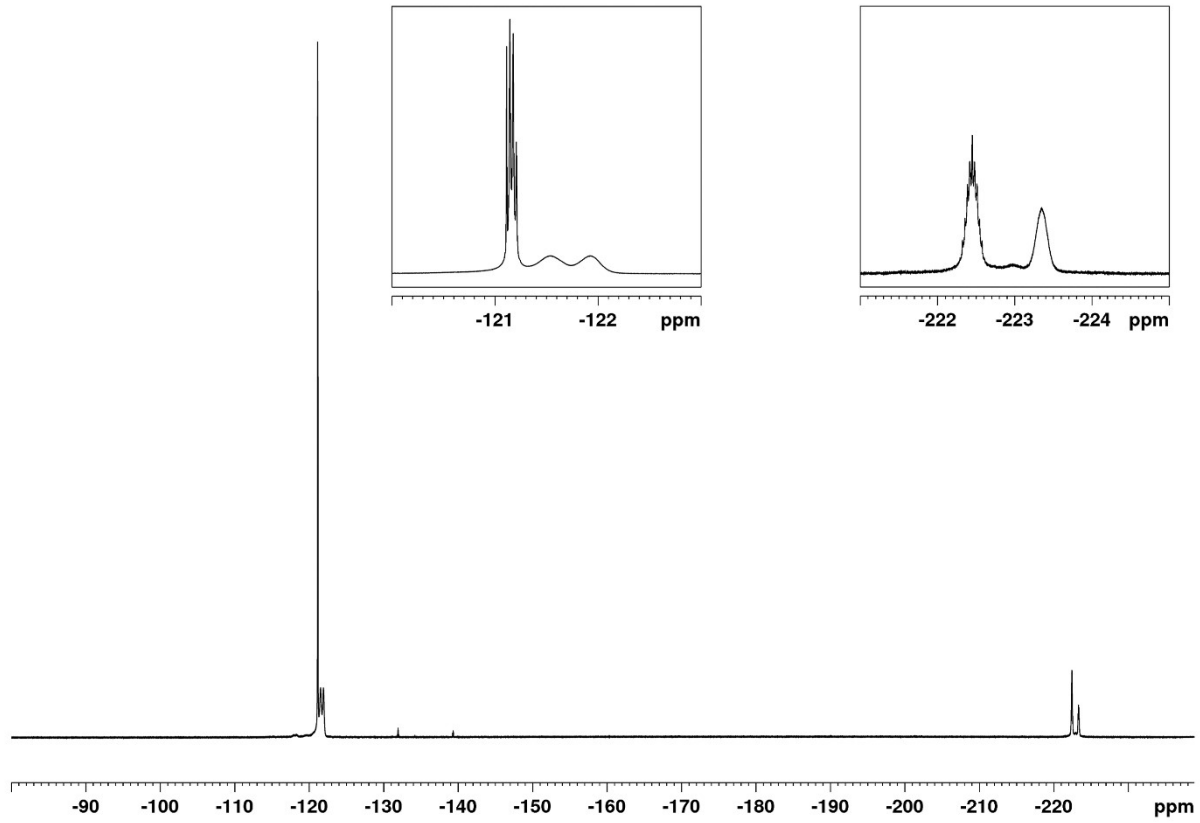


Figure S- 69: ^{19}F-NMR (188.31 MHz, 298 K, CH_2Cl_2) of [NO][Al($OC_{10}F_{15}$)$_4$] and P_4 in CH_2Cl_2.

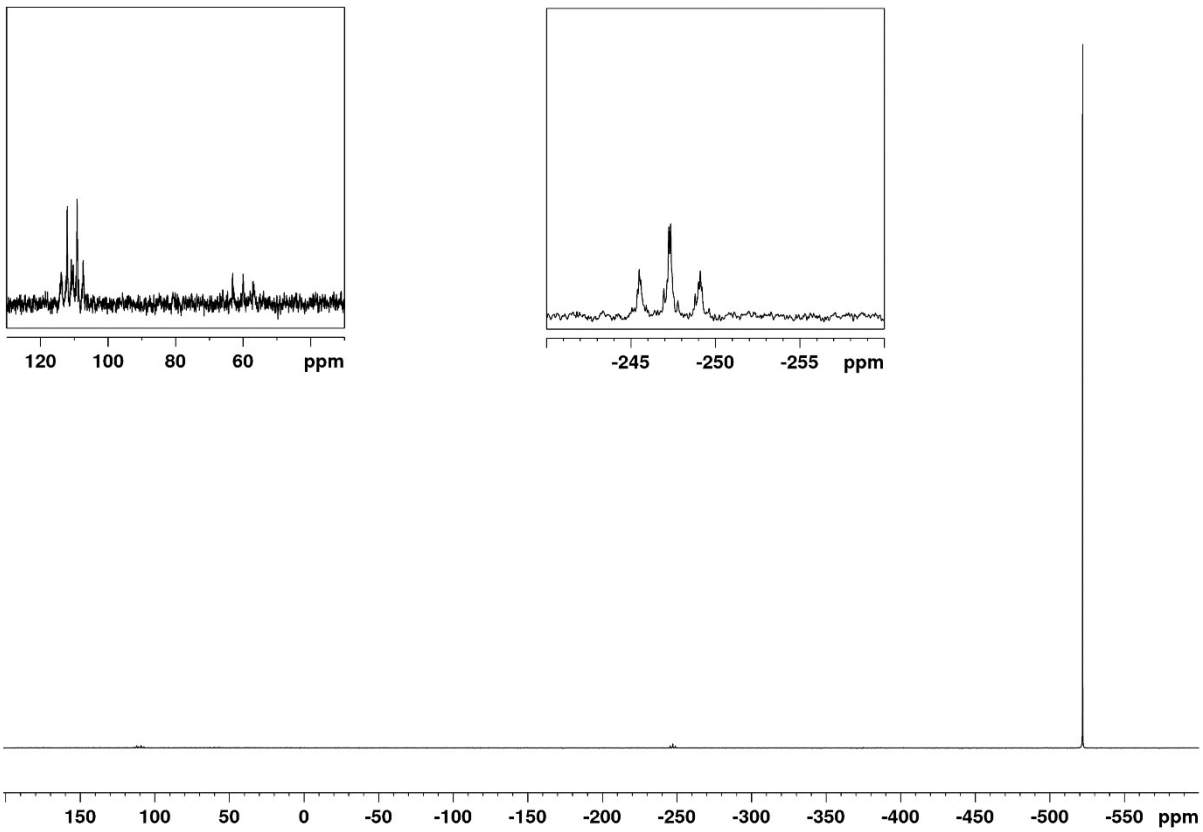


Figure S- 70: ^{31}P-NMR (81.01 MHz, 298 K, CH_2Cl_2) of [NO][Al($OC_{10}F_{15}$)$_4$] and P_4 in CH_2Cl_2.

Synthesis of $Tl[Al(OC_{10}F_{15})_4]$ containing impurities of $C_{10}F_{15}OH/C_{10}F_{15}O^-$

$Li[Al(OC_{10}F_{15})_4]$ (0.610 g, 0.355 mmol) containing impurities of alcohol $C_{10}F_{15}OH$ and $TlNO_3$ (0.209 g, 0.785 mmol, 2.21 eq.) were dissolved in *o*-DFB (6.0 mL), acetone (0.5 mL) and H_2O (0.5 mL) and stirred at room temperature overnight. Additional H_2O (20 mL) was added to dissolve the occurred colorless solid. The reaction solution was sonicated for 4 h. The organic phase was separated, washed with H_2O (3x 5 mL) and the solvents removed under reduced pressure. The obtained colorless solid (0.442 g, 0.231 mmol, 65 %) was analyzed by NMR spectroscopy showing impurities of alcoholate and only traces of Li^+.

The colorless solid was dissolved in *o*-DFB (1.5 mL) and crystallized with *n*-pentane. Initially, only amorphous solid precipitated, but after another few days, the formation of crystals could be observed, which were examined by NMR and IR spectroscopy and single crystal X-ray diffraction. Since the obtained crystals are embedded in the amorphous solid, it was hard to separate larger amounts of crystals from the rest and therefore not a suitable purification method.

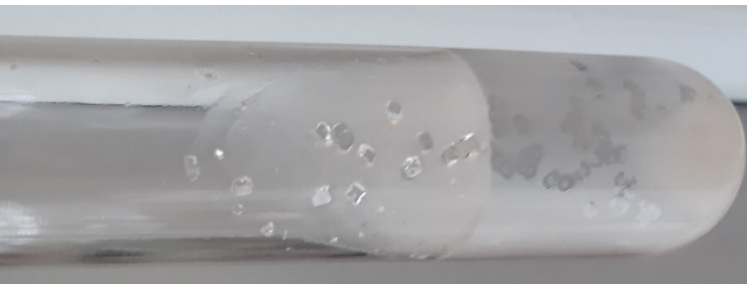


Figure S- 71: Crystals of $Tl[Al(OC_{10}F_{15})_4]$ embedded in amorphous $Tl[Al(OC_{10}F_{15})_4]$ further containing impurities of alcohol/alcoholate.

NMR data before crystallization:

^{1}H-NMR (400.17 MHz, 298 K, *o*-DFB): δ = 2.31 (br. s, 6H, acetone) ppm.
^{7}Li-NMR (155.52 MHz, 298 K, *o*-DFB): δ = 2.1 (Li^+, $LiOC_{10}F_{15}$ or $Li[Al(OC_{10}F_{15})_4]$) ppm.
^{19}F-NMR (282.45 MHz, 298 K, *o*-DFB): δ = −223.2 (m, C**F**, 12F, $Tl[Al(OC_{10}F_{15})_4]$), −222.8 (m, C**F**, 3F, $C_{10}F_{15}OH/C_{10}F_{15}O^-$), −121.3 (m, C**F$_2$**, 48F, $Tl[Al(OC_{10}F_{15})_4]$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, *o*-DFB): δ = 35.4 (s, 1Al, $Tl[$**Al**$(OC_{10}F_{15})_4]$) ppm.

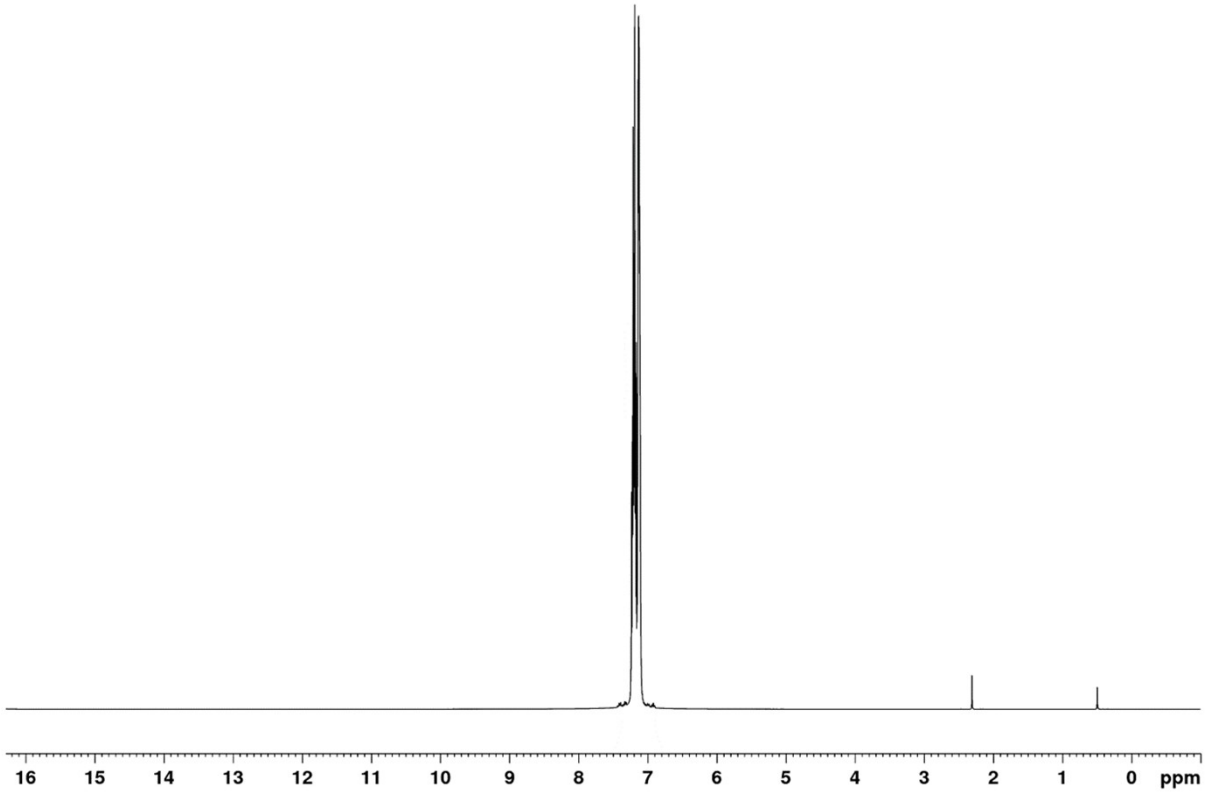


Figure S- 72: ^{1}H-NMR spectrum (400.17 MHz, 298 K, *o*-DFB) of Tl[Al(OC$_{10}$F$_{15}$)$_4$] of the obtained colorless solid before crystallization.

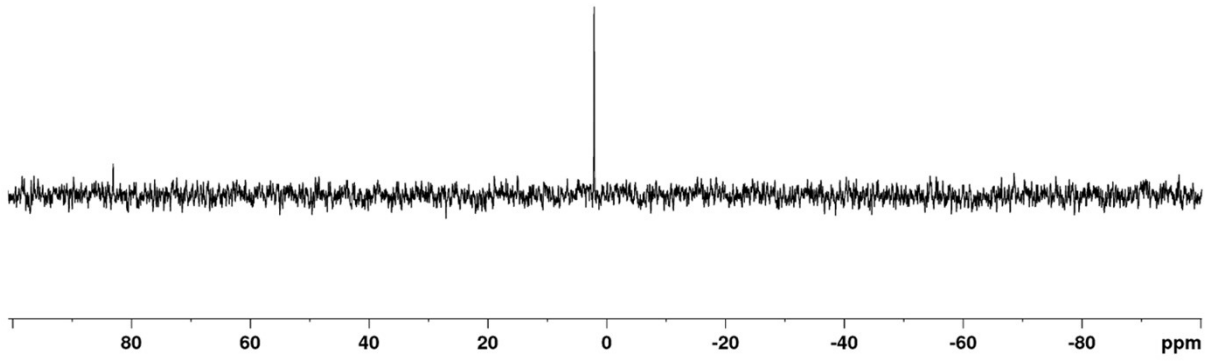


Figure S- 73: ^{7}Li-NMR spectrum (155.52 MHz, 298 K, *o*-DFB) of Tl[Al(OC$_{10}$F$_{15}$)$_4$] of the obtained colorless solid before crystallization showing only traces of Li^{+}.

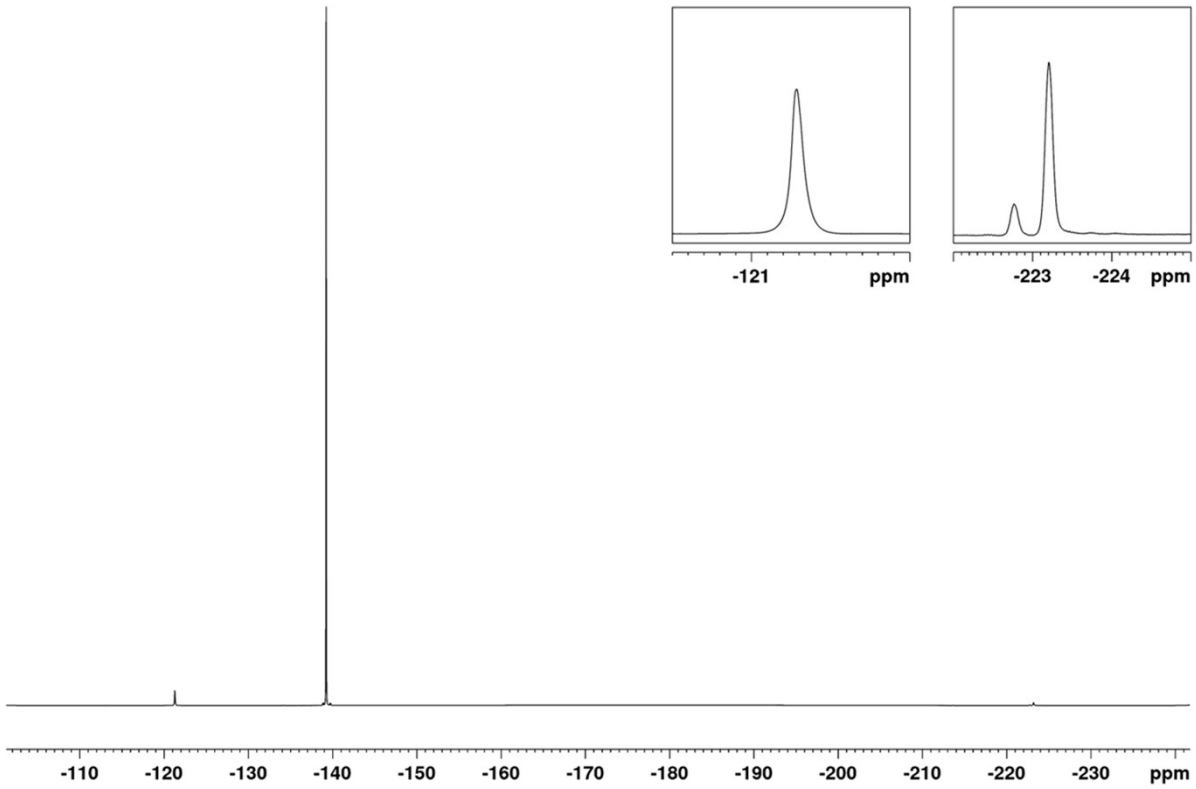


Figure S- 74: ^{19}F-NMR spectrum (282.45 MHz, 298 K, *o*-DFB) of Tl[Al(OC$_{10}$F$_{15}$)$_4$] of the obtained colorless solid before crystallization.

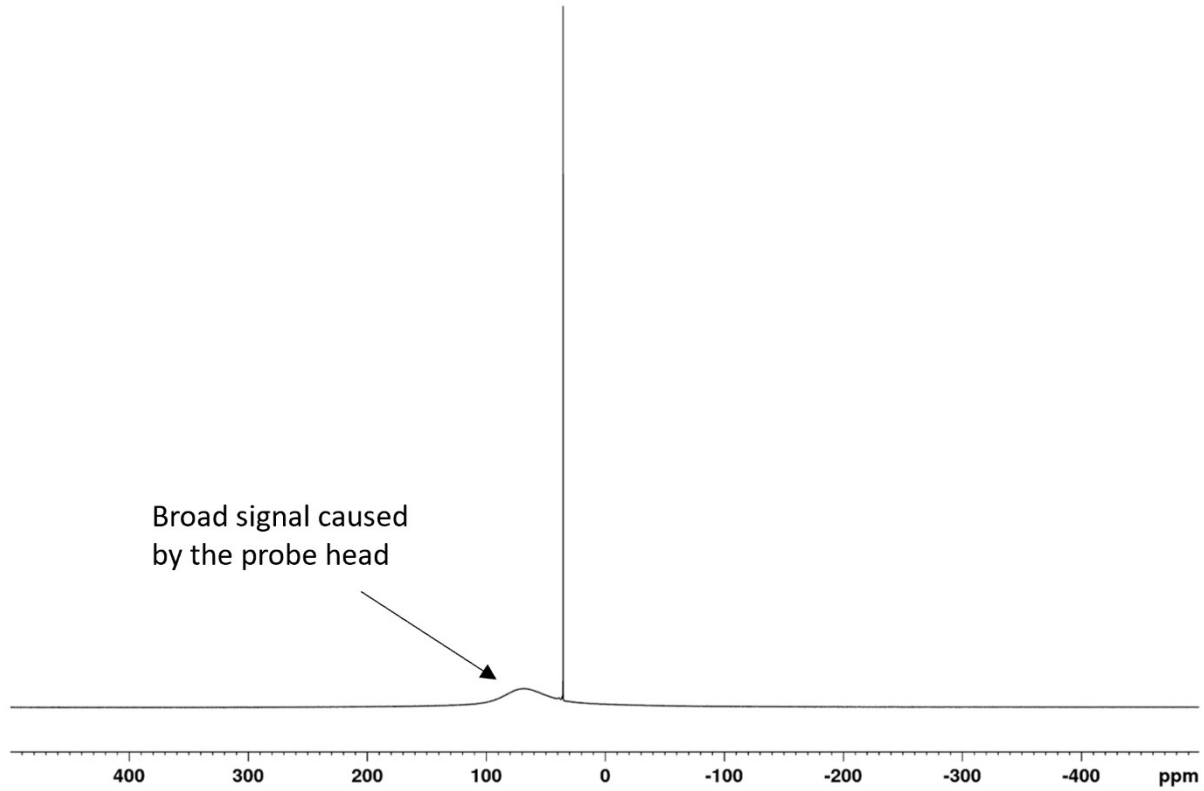


Figure S- 75: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, *o*-DFB) of Tl[Al(OC$_{10}$F$_{15}$)$_4$] of the obtained colorless solid before crystallization.

NMR and IR data after crystallization:

^{1}H-NMR (400.17 MHz, 298 K, CD_2Cl_2): δ = 2.15 (br. s, 6H, acetone) ppm.

^{7}Li-NMR (155.52 MHz, 298 K, CD_2Cl_2): no signal.

^{19}F-NMR (376.54 MHz, 298 K, CD_2Cl_2): δ = −223.4 (m, C**F**, 12F, Tl[Al($OC_{10}F_{15}$)$_4$]), −121.8 (m, C**F_2**, 48F, Tl[Al($OC_{10}F_{15}$)$_4$]) ppm.

^{27}Al-NMR (104.27 MHz, 298 K, CD_2Cl_2): δ = 34.7 (s, 1Al, Tl[**Al**($OC_{10}F_{15}$)$_4$]) ppm.

FTIR (Diamant, ATR): $\tilde{\nu}$ = 1697 (vw), 1686 (vw), 1350 (vw), 1292 (w), 1268 (vs), 1109 (vw), 979 (s), 954 (vs), 762 (vw), 678 (w), 651 (w), 643 (vw), 533 (vw), 441 (m), 402 (w) cm^{-1}.

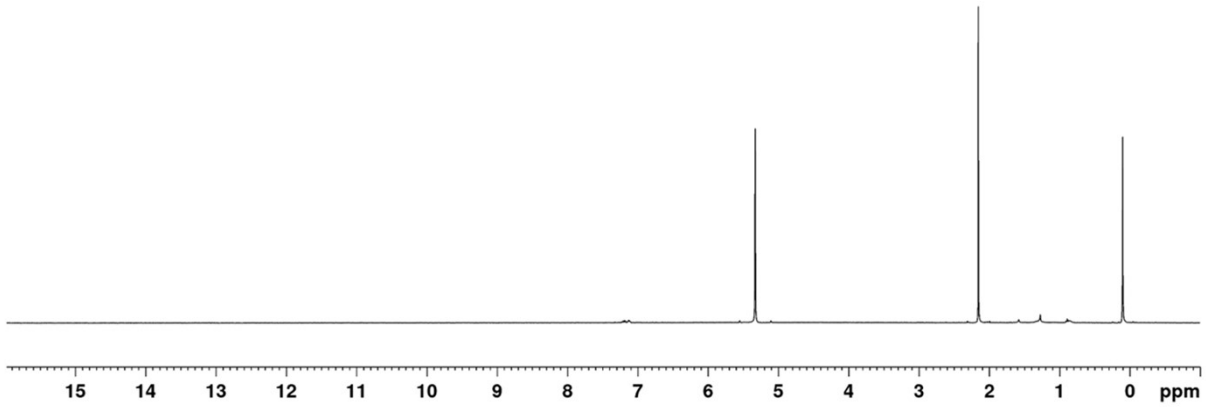


Figure S- 76: ^{1}H-NMR spectrum (400.17 MHz, 298 K, CD_2Cl_2) of Tl[Al($OC_{10}F_{15}$)$_4$] of the obtained colorless crystals.

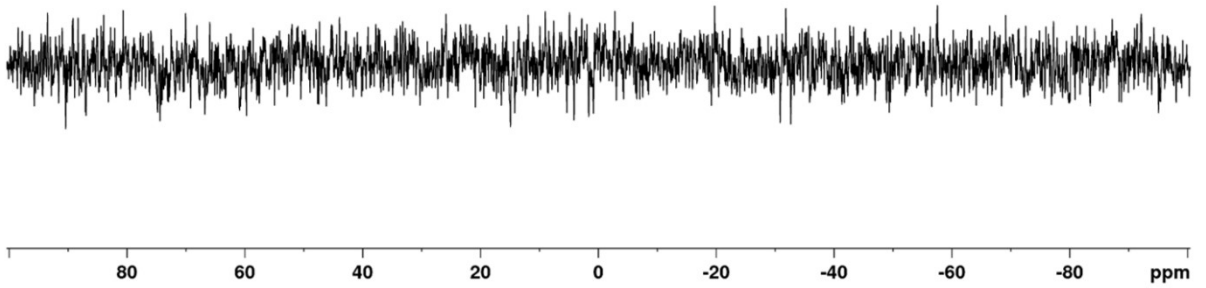


Figure S- 77: ^{7}Li-NMR spectrum (155.52 MHz, 298 K, CD_2Cl_2) of Tl[Al($OC_{10}F_{15}$)$_4$] of the obtained colorless crystals. → Li^+ is absent.

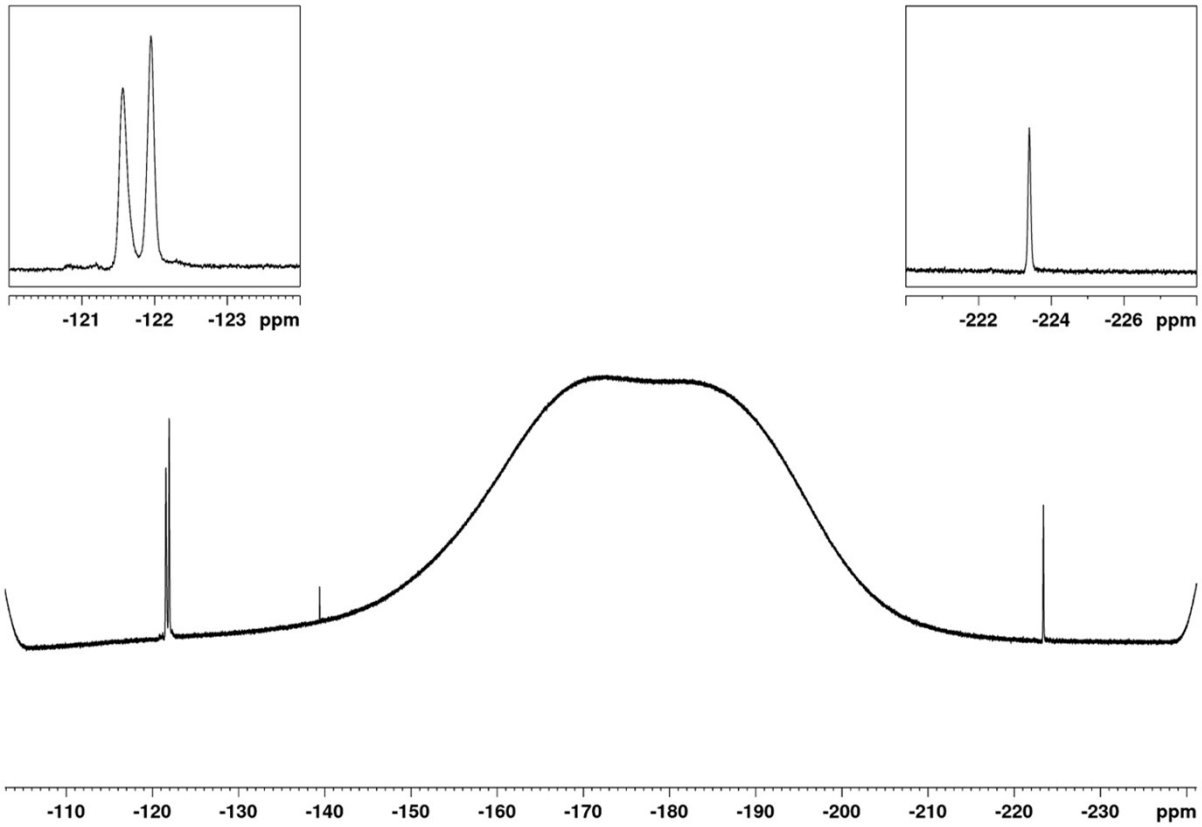


Figure S- 78: ^{19}F-NMR spectrum (376.54 MHz, 298 K, CD_2Cl_2) of $Tl[Al(OC_{10}F_{15})_4]$ of the obtained colorless crystals.

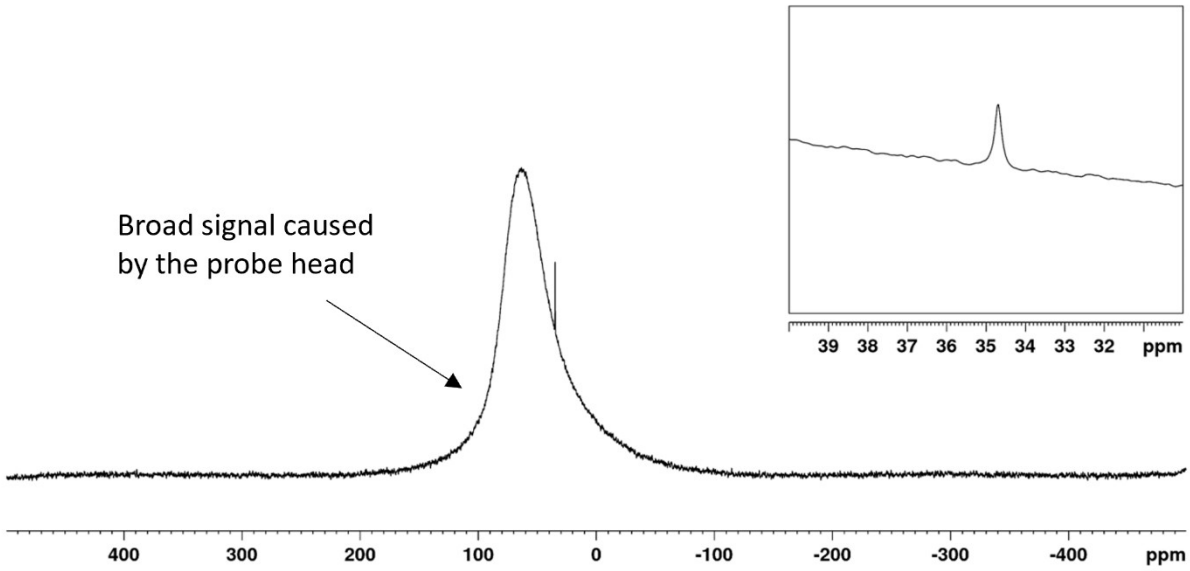


Figure S- 79: ^{27}Al-NMR spectrum (104.27 MHz, 298 K, CD_2Cl_2) of $Tl[Al(OC_{10}F_{15})_4]$ of the obtained colorless crystals.

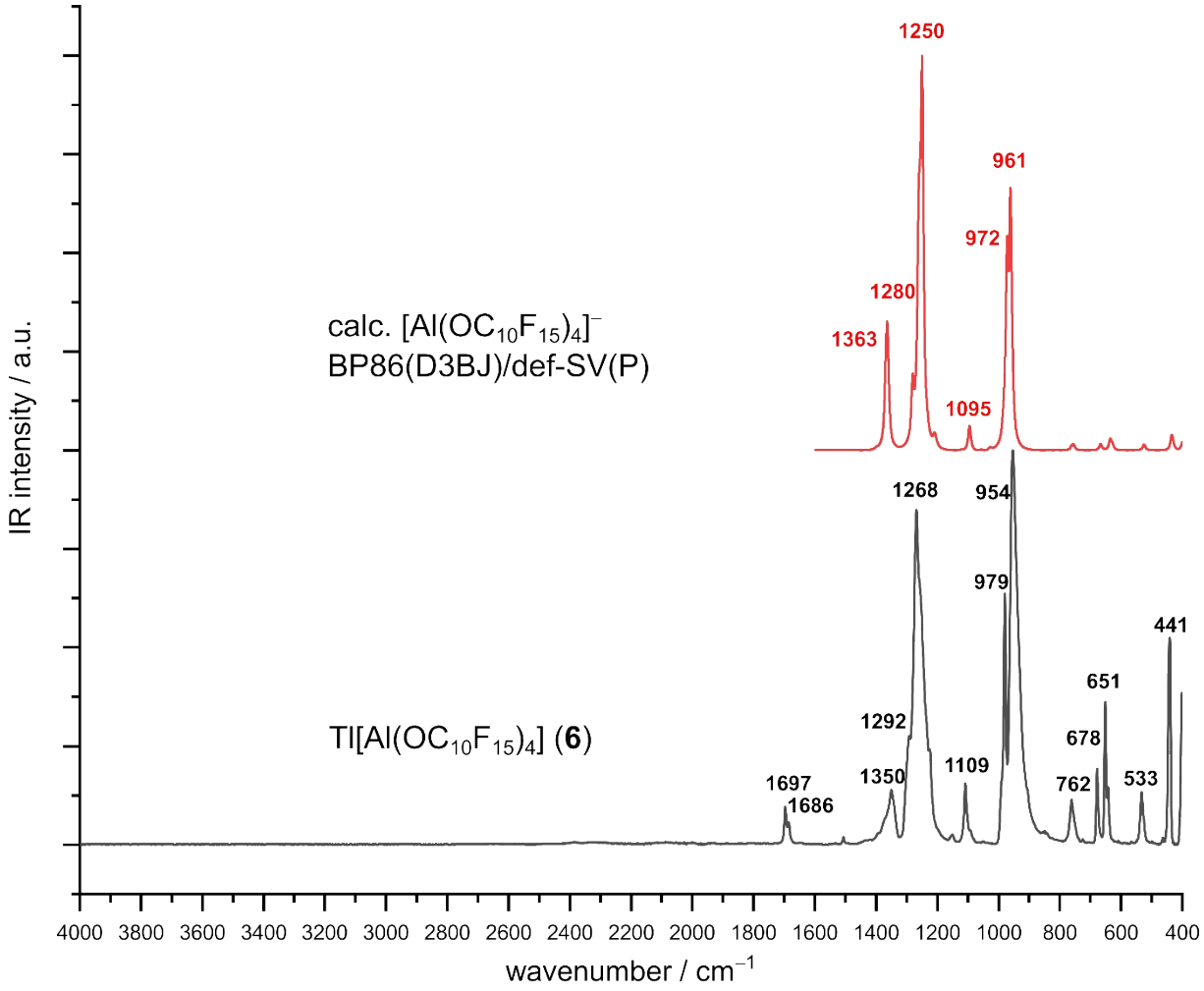


Figure S- 80: IR spectrum of Tl[Al(OC$_{10}$F$_{15}$)$_4$] (black) in comparison with the calculated IR spectrum of the [*pfAd*]$^-$ anion at BP86(D3BJ)/def-SV(P) level of theory (red). All IR data of obtained pure substances of the [*pfAd*]$^-$ anion are compared and assigned in Table S- 1.

Synthesis of [H(Et$_2$O)$_2$][Al(OC$_{10}$F$_{15}$)$_4$]

Starting from unpurified Li[Al(OC$_{10}$F$_{15}$)$_4$]

Li[Al(OC$_{10}$F$_{15}$)$_4$] (2.84 g, 1.65 mmol) containing impurities of alcohol C$_{10}$F$_{15}$OH and a solution of HCl in Et$_2$O (2 M, 40 mL, 80.0 mmol) were stirred for five days at r.t. The solvent was removed under reduced pressure. The target compound was extracted with *o*-DFB (3x 25 mL) and the solvent was removed afterwards under reduced pressure. The solid residue (2.31 g) was washed with CH$_2$Cl$_2$ (4x 10 mL), dried under reduced pressure and the colorless solid (1.99 g, 1.07 mmol, 65 %) analyzed by NMR and IR spectroscopy. Additional, suitable crystals for s-XRD could be obtained by storage of [H(Et$_2$O)$_2$][Al(OC$_{10}$F$_{15}$)$_4$] in *o*-DFB at −40 °C.

^{1}H-NMR (300.18 MHz, 298 K, *o*-DFB): δ = 1.63 (t, C**H$_3$**, 12H, [H(Et$_2$O)$_2$][Al(OC$_{10}$F$_{15}$)$_4$]), 4.27 (q, C**H$_2$**, 8H, [H(Et$_2$O)$_2$][Al(OC$_{10}$F$_{15}$)$_4$]), 16.20 (br. s, 1H, [**H**(Et$_2$O)$_2$][Al(OC$_{10}$F$_{15}$)$_4$]) ppm.
^{7}Li-NMR (116.66 MHz, 298 K, *o*-DFB): δ = −0.1 (br. s, 1Li, Li$^+$) ppm, only traces.
^{19}F-NMR (282.45 MHz, 298 K, *o*-DFB): δ = −223.2 (m, C**F**, 12F, [H(Et$_2$O)$_2$][Al(OC$_{10}$F$_{15}$)$_4$]), −121.3 (m, C**F$_2$**, 48F, [H(Et$_2$O)$_2$][Al(OC$_{10}$F$_{15}$)$_4$]) ppm.

^{27}Al-NMR (78.22 MHz, 298 K, *o*-DFB): δ = 35.4 (s, 1Al, $[H(Et_2O)_2][\mathbf{Al}(OC_{10}F_{15})_4]$) ppm.

FTIR (Diamant, ATR): $\tilde{\nu}$ = 1392 (vw), 1353 (vw), 1295 (vw), 1269 (vs), 1255 (m), 1192 (vw), 1108 (vw), 1016 (vw), 981 (m), 955 (vs), 905 (w), 760 (vw), 679 (vw), 652 (w), 533 (vw), 443 (w), 402 (w) cm^{-1}.

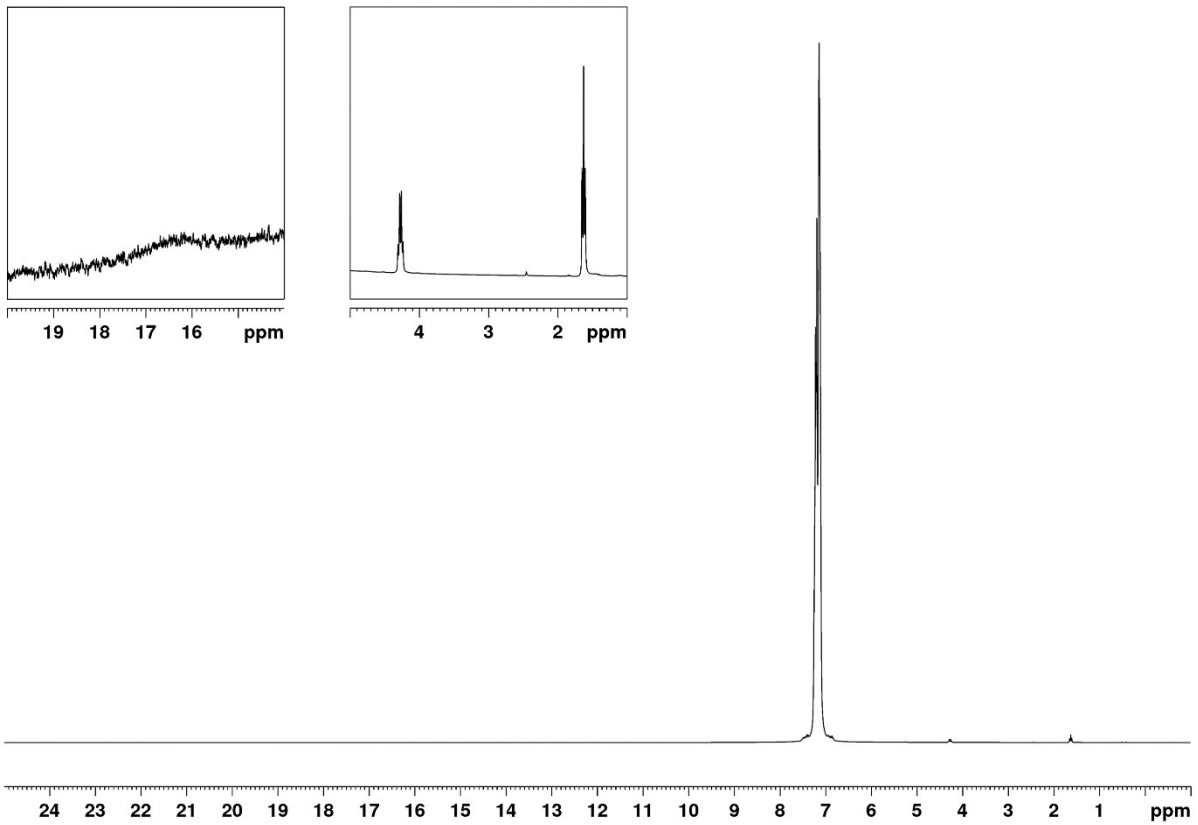


Figure S- 81: ^{1}H-NMR spectrum (300.18 MHz, 298 K, *o*-DFB) of $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$.

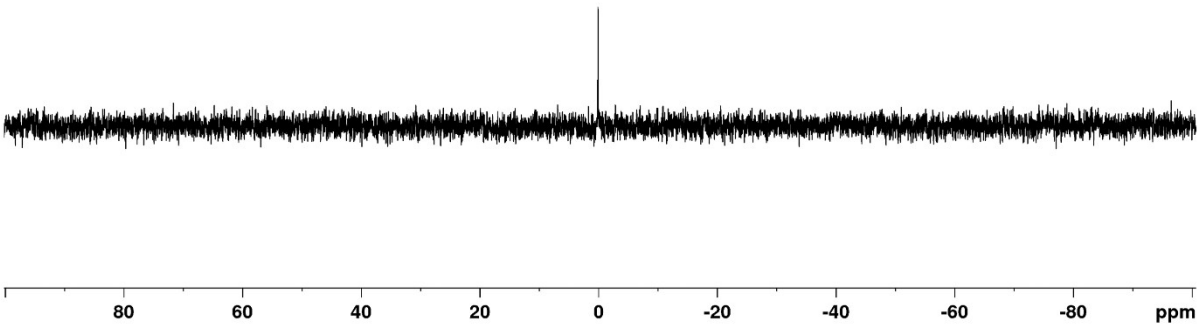


Figure S- 82: ^{7}Li-NMR spectrum (116.66 MHz, 298 K, *o*-DFB) of $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$. -> only traces!

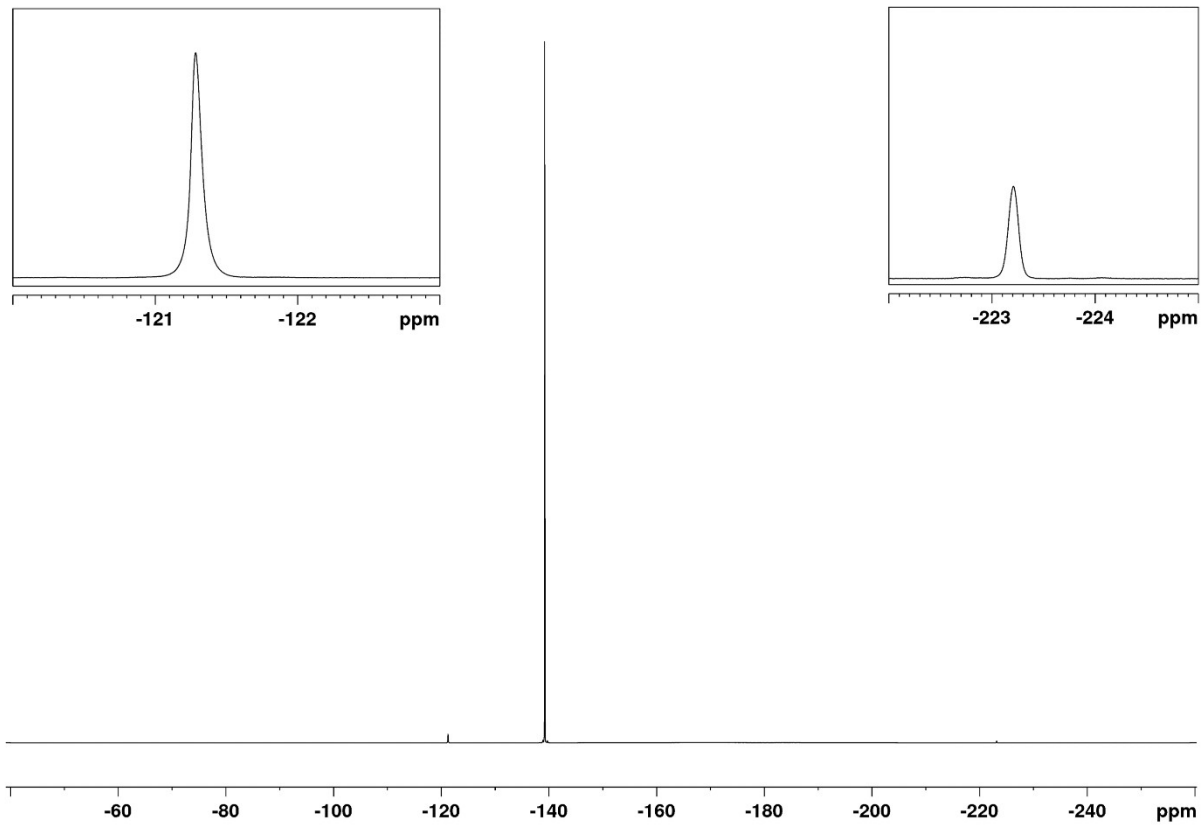


Figure S- 83: ^{19}F-NMR spectrum (282.45 MHz, 298 K, *o*-DFB) of $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$.

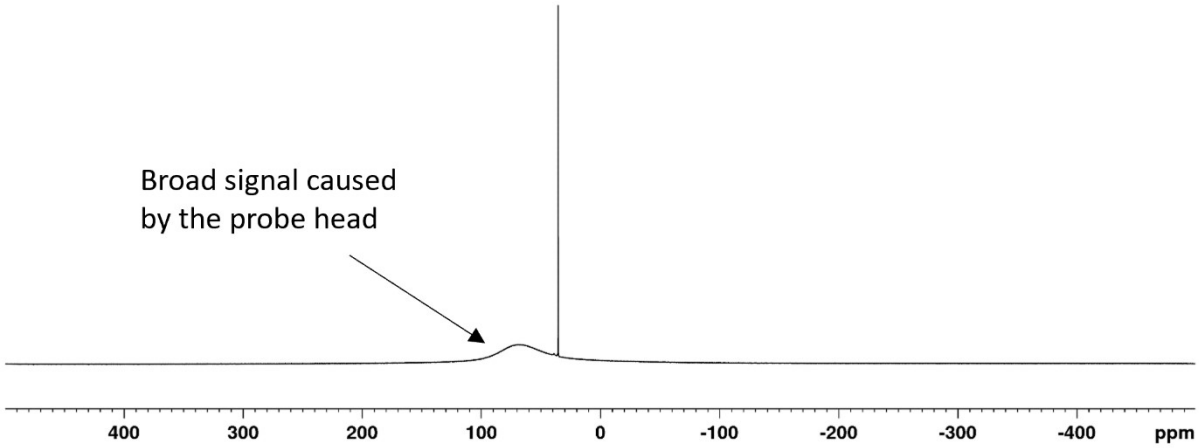


Figure S- 84: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, *o*-DFB) of $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$.

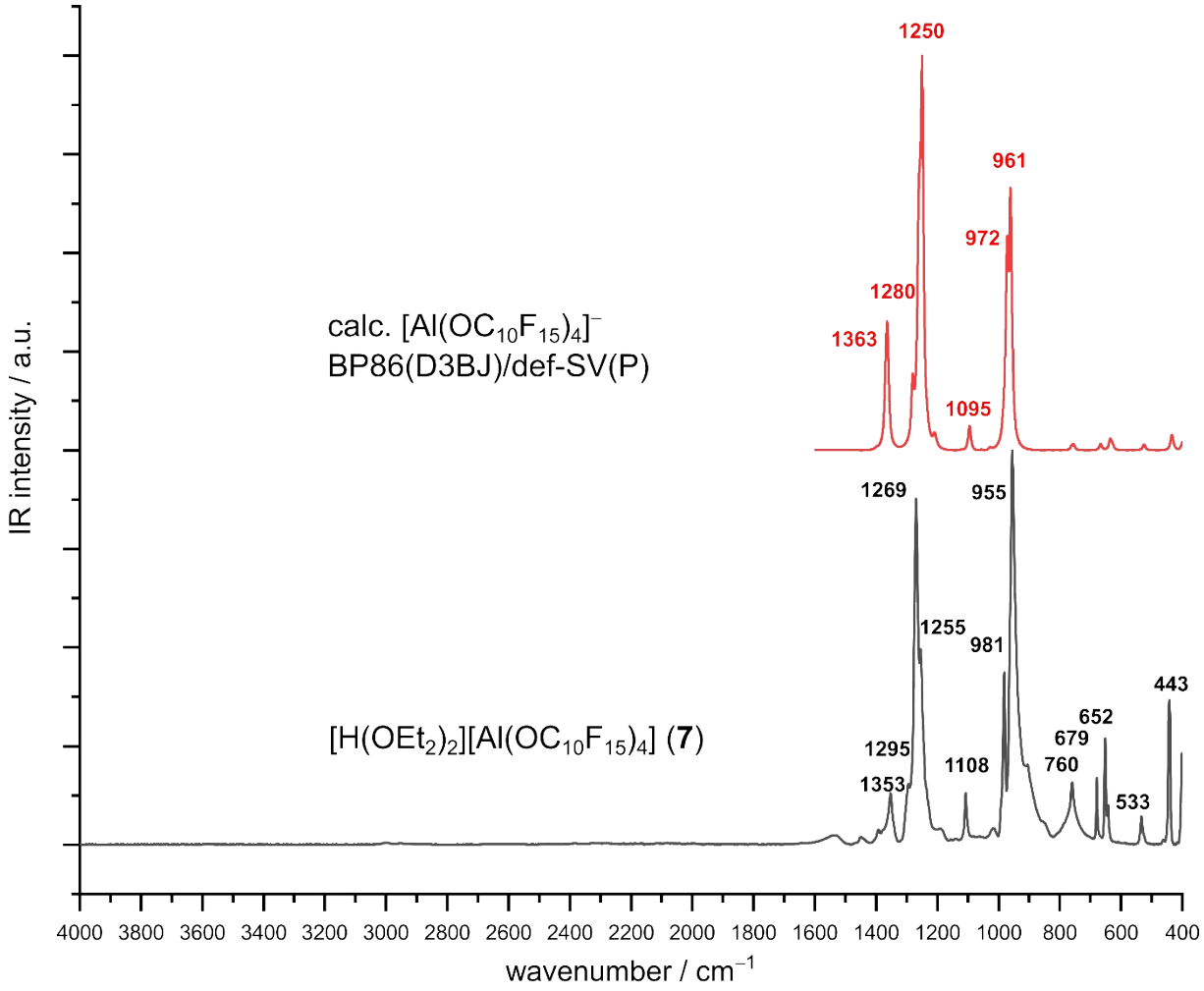


Figure S- 85: IR spectrum of $[H(OEt_2)_2][Al(OC_{10}F_{15})_4]$ (black) in comparison with the calculated IR spectrum of the [*pfAd*]$^-$ anion at BP86(D3BJ)/def-SV(P) level of theory (red). All IR data of obtained pure substances of the [*pfAd*]$^-$ anion are compared and assigned in Table S- 1.

Starting from unpurified $Na[Al(OC_{10}F_{15})_4]$

$Na[Al(OC_{10}F_{15})_4]$ (0.90 g, 0.52 mmol) containing impurities of alcohol $C_{10}F_{15}OH$ was suspended in CH_2Cl_2 (6.0 mL). A solution of HCl in Et_2O (2 M, 15 mL, 30.0 mmol) was added and the reaction mixture was stirred for three days at r.t. The solvent was removed under reduced pressure. The target compound was extracted with *o*-DFB (15 mL) and the solvent was removed afterwards under reduced pressure. The solid residue was washed with CH_2Cl_2 (2x 10 mL), dried under reduced pressure and the colorless solid (0.483 g, 0.259 mmol, 50 %) analyzed by NMR spectroscopy.

^{1}H-NMR (300.18 MHz, 298 K, *o*-DFB): δ = 1.63 (t, C**H$_3$**, 12H, $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$), 4.29 (q, C**H$_2$**, 8H, $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$), 16.53 (br. s, 1H, [**H**$(Et_2O)_2][Al(OC_{10}F_{15})_4]$) ppm.

^{19}F-NMR (282.45 MHz, 298 K, *o*-DFB): δ = −223.2 (m, C**F**, 12F, $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$), −121.3 (m, C**F$_2$**, 48F, $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$) ppm.

^{23}Na-NMR (79.40 MHz, 298 K, *o*-DFB): no signal (as expected)

^{27}Al-NMR (78.22 MHz, 298 K, *o*-DFB): δ = 35.3 (s, 1Al, $[H(Et_2O)_2][$**Al**$(OC_{10}F_{15})_4]$) ppm.

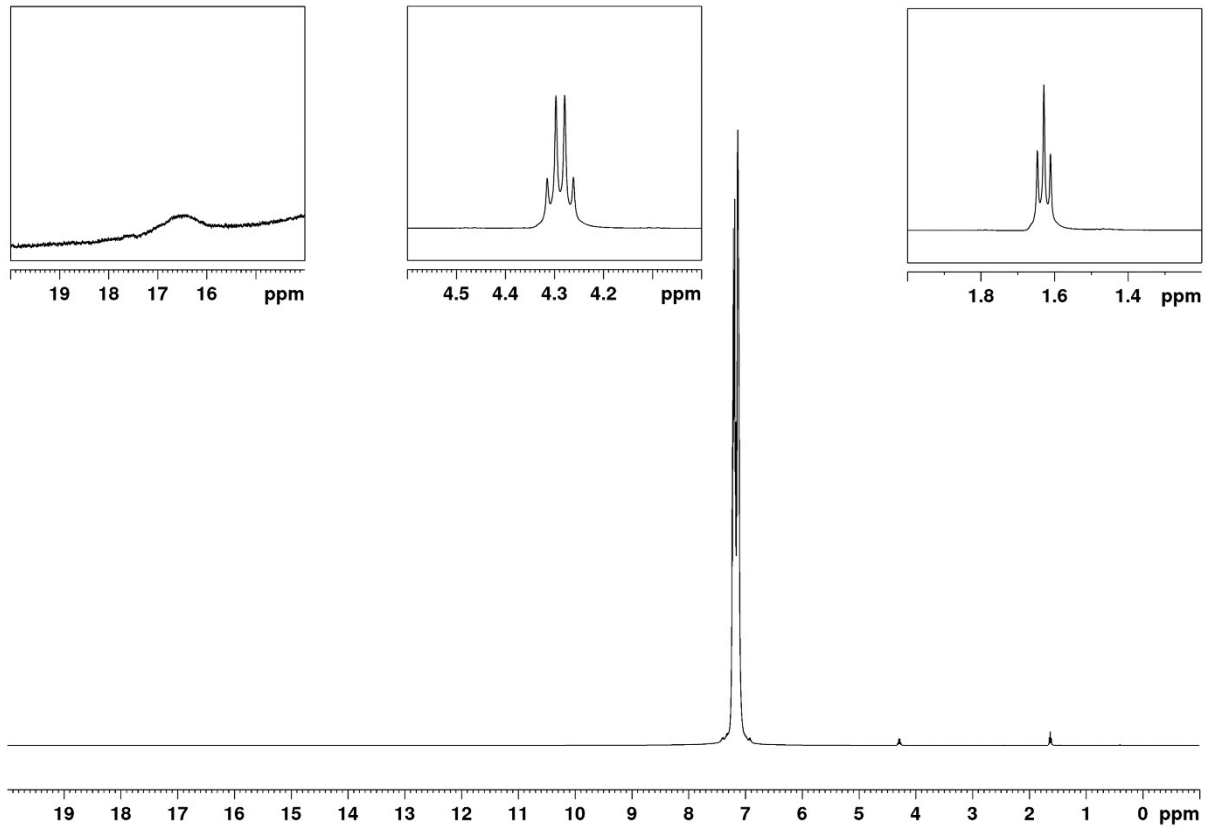


Figure S- 86: ^{1}H-NMR spectrum (400.17 MHz, 298 K, *o*-DFB) of $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$ from $NaAl(OC_{10}F_{15})_4$.

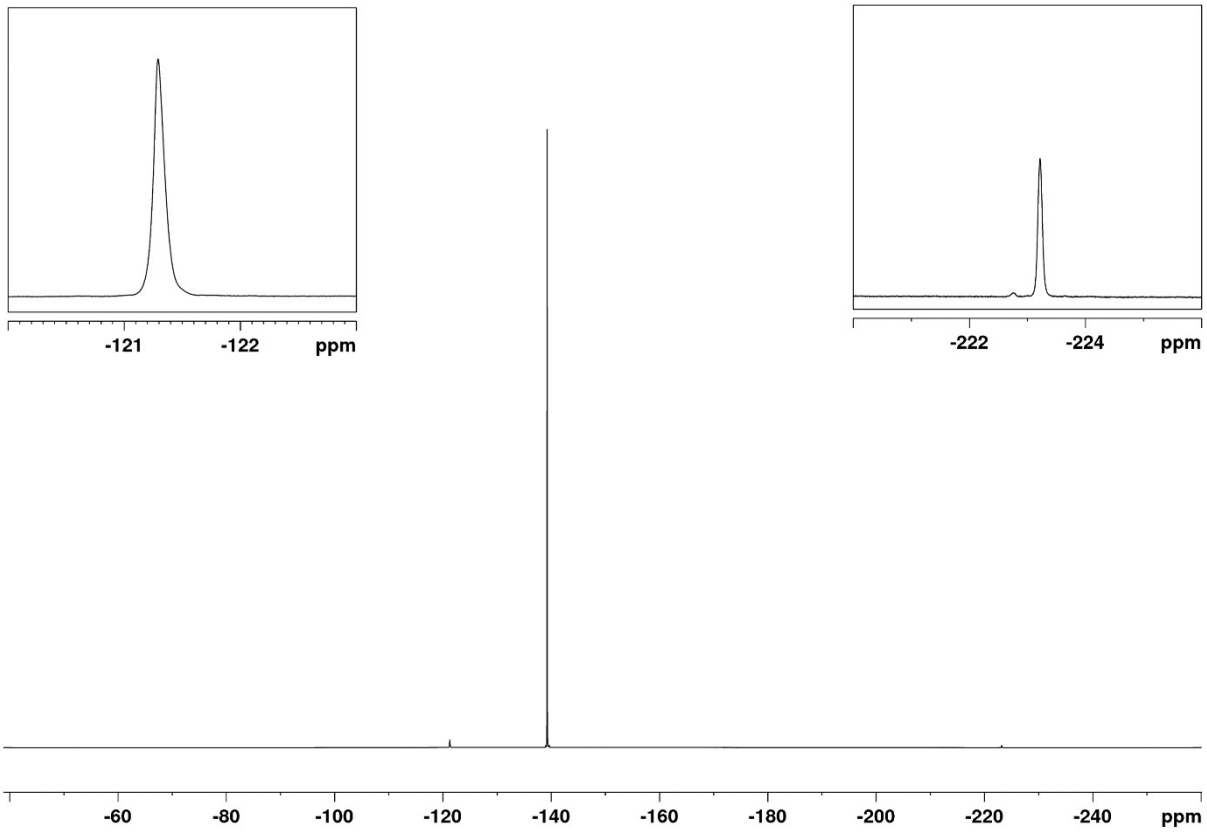


Figure S- 87: ^{19}F-NMR spectrum (376.54 MHz, 298 K, *o*-DFB) of $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$ from $NaAl(OC_{10}F_{15})_4$.

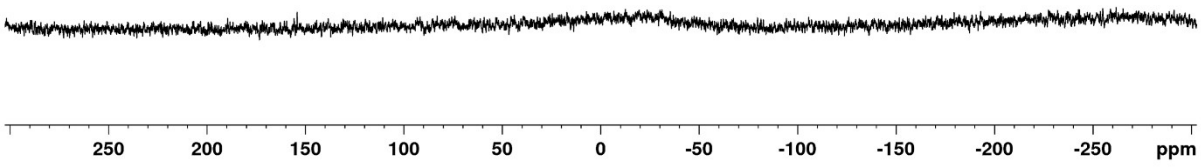


Figure S- 88: ^{23}Na-NMR spectrum (79.40 MHz, 298 K, *o*-DFB) of $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$ from $NaAl(OC_{10}F_{15})_4$.

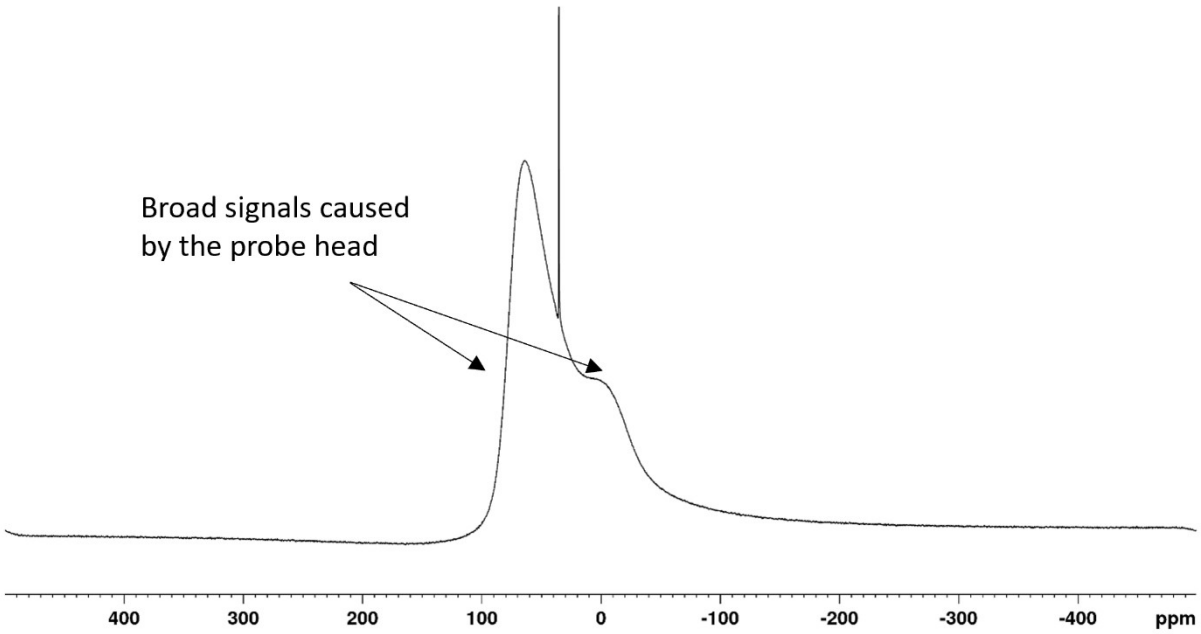


Figure S- 89: ^{27}Al-NMR spectrum (104.27 MHz, 298 K, *o*-DFB) of $[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$ from $NaAl(OC_{10}F_{15})_4$.

Synthesis of $Li[Al(OC_{10}F_{15})_4]\cdot(Et_2O)_2$

$[H(Et_2O)_2][Al(OC_{10}F_{15})_4]$ (1.31 g, 0.759 mmol) and LiHMDS (0.127 g, 0.759 mmol, 1.0 eq) were submitted into a Schlenk flask, suspended in *o*-DFB (7.0 mL) and stirred for 2.5 h at r.t. The solvent was removed under reduced pressure, the solid residue was washed with toluene (3x 5.0 mL) and dried under reduced pressure for several hours. The target compound was obtained as colorless solid (1.22 g, 0.681 mmol, 90 %) and analyzed by NMR spectroscopy.

^{1}H-NMR (300.18 MHz, 298 K, THF): δ = 1.07 (t, 6H, $CH_3CH_2OCH_2CH_3$), 3.30 (q expected, hard to distinguish from the THF resonance, 4H, $CH_3CH_2OCH_2CH_3$) ppm.
^{7}Li-NMR (116.66 MHz, 298 K, THF): δ = −0.3 (br. s, 1Li, Li^+) ppm.
^{19}F-NMR (282.45 MHz, 298 K, THF): δ = −224.0 (m, C**F**, 12F, $Li[Al(OC_{10}F_{15})_4]$), −122.0 (m, CF_2, 48F, $Li[Al(OC_{10}F_{15})_4]$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, THF): δ = 34.6 (s, 1Al, $Li[Al(OC_{10}F_{15})_4]$) ppm.

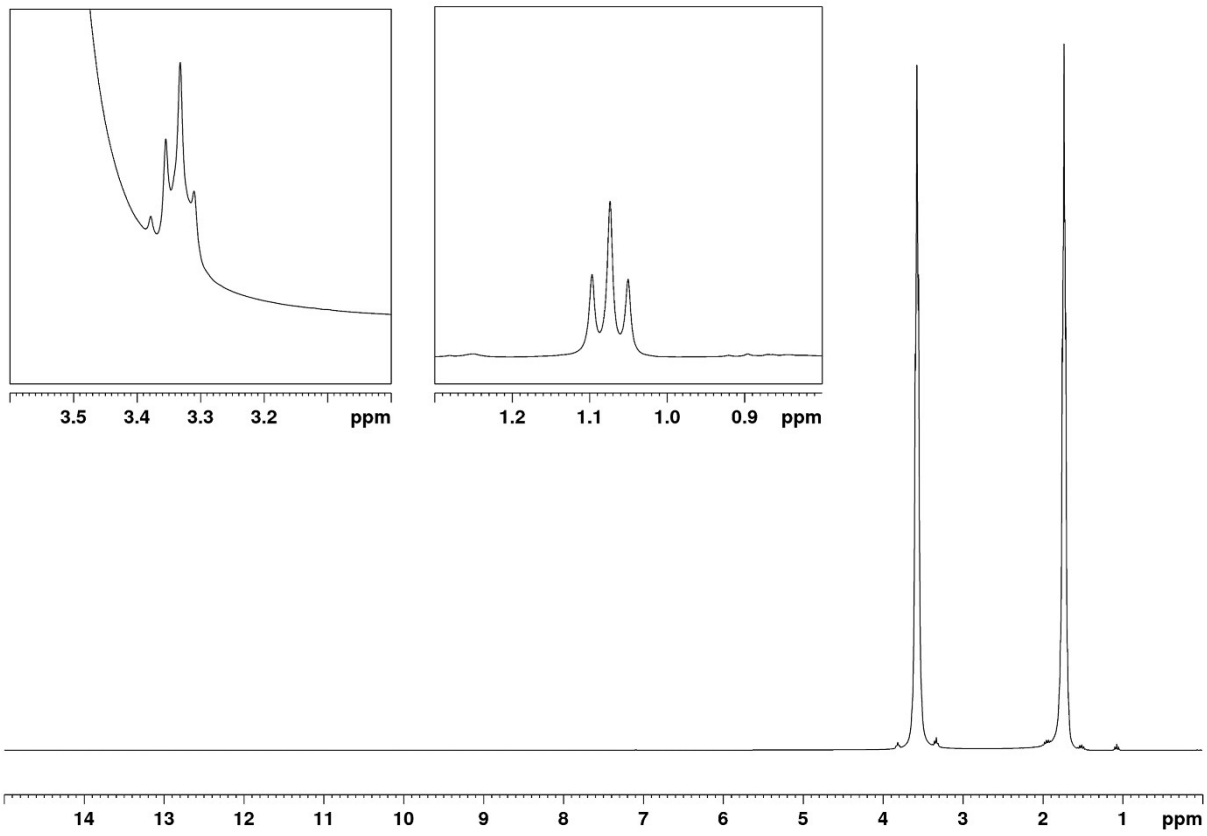


Figure S- 90: ^{1}H-NMR (300.18 MHz, 298 K, THF) of $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$.

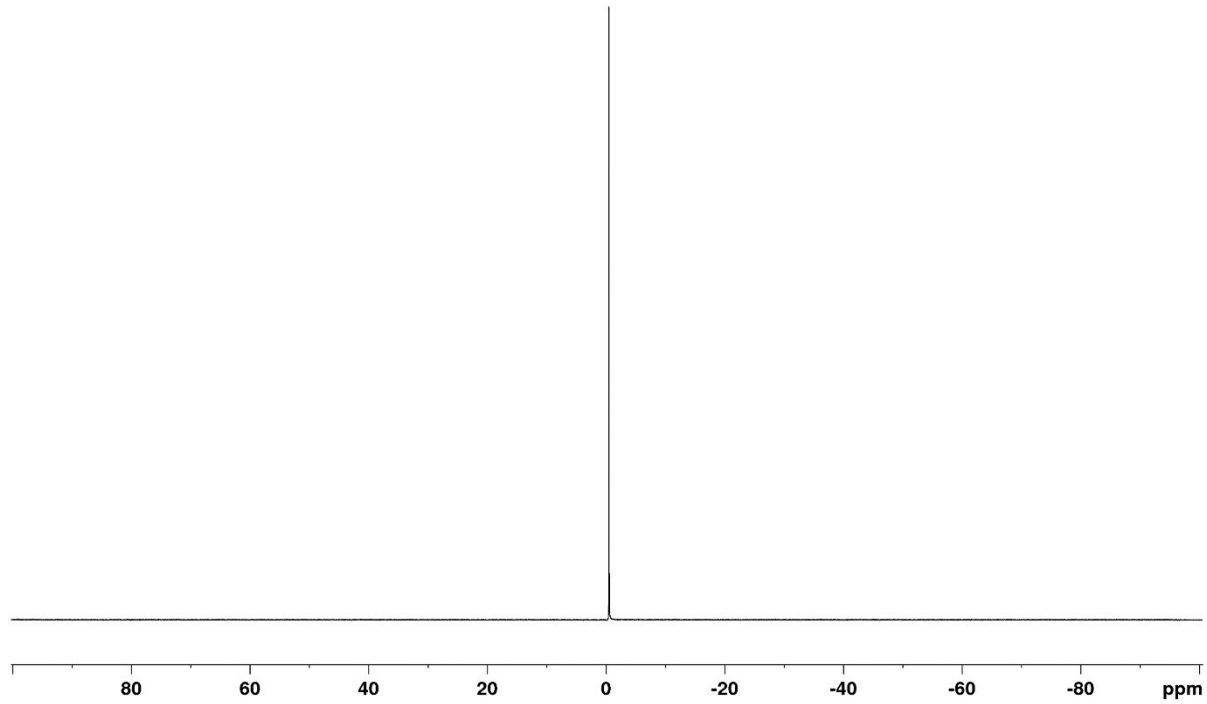


Figure S- 91: ^{7}Li-NMR (116.66 MHz, 298 K, THF) of $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$.

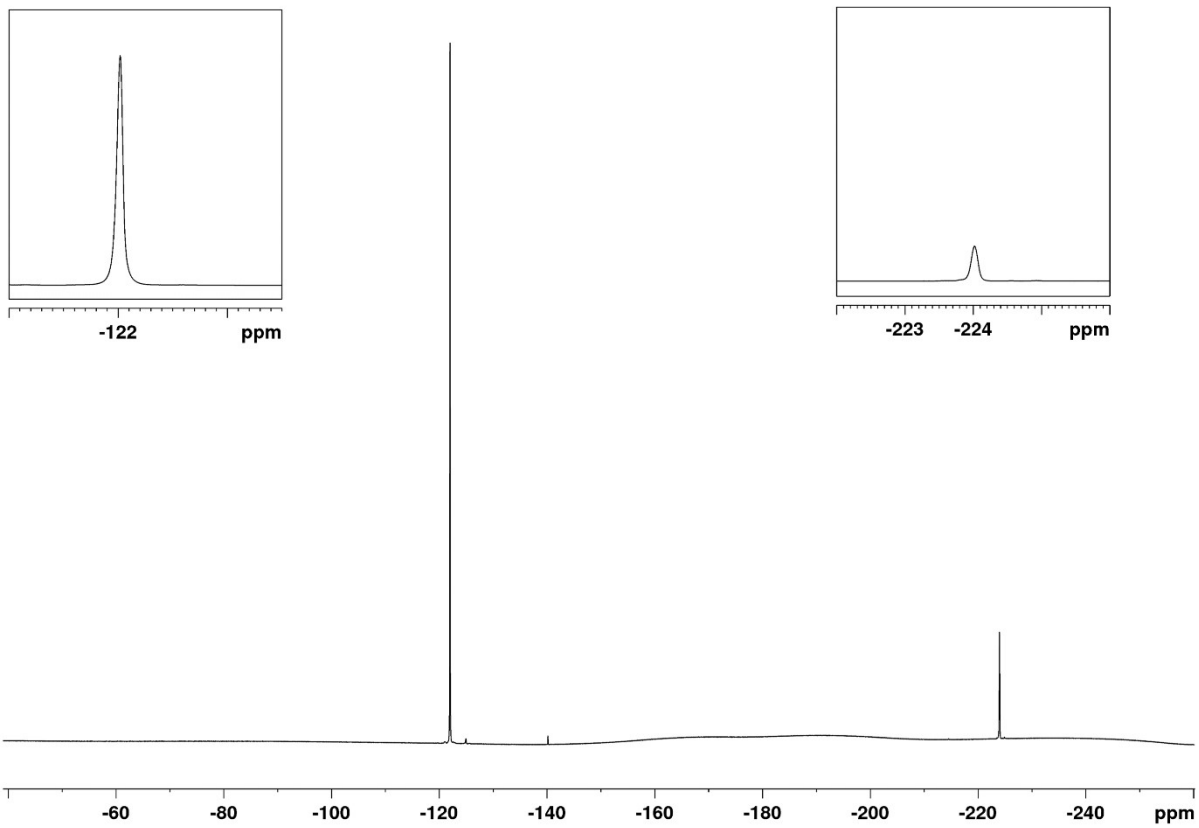


Figure S- 92: ^{19}F-NMR (282.45 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$]·2Et$_2$O.

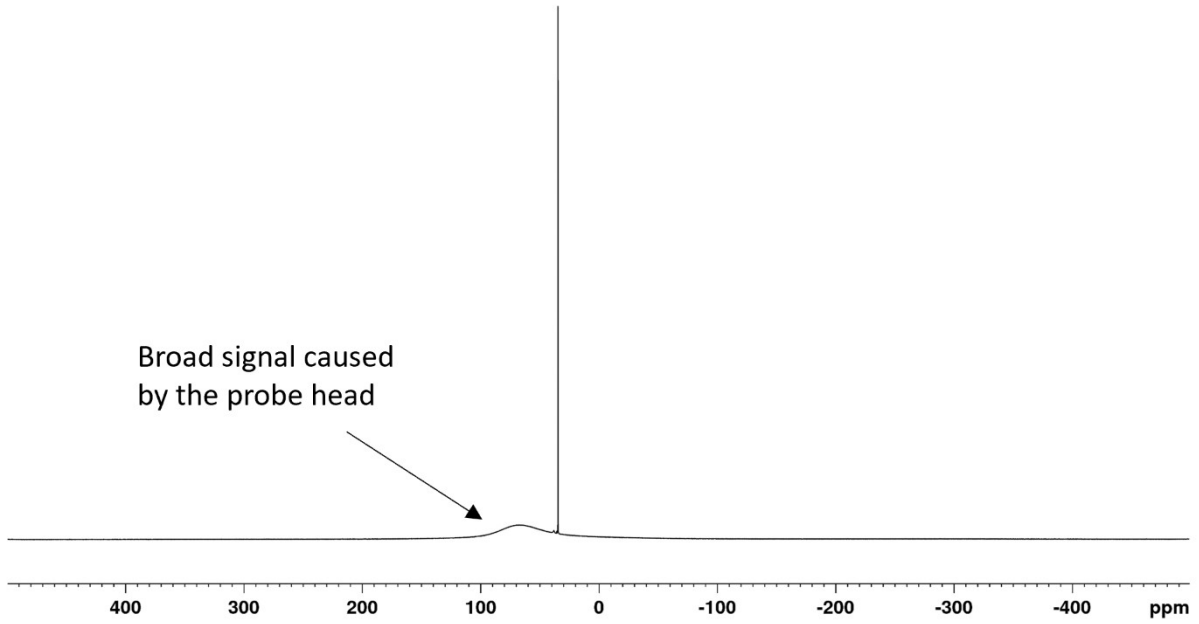


Figure S- 93: ^{27}Al-NMR (78.22 MHz, 298 K, THF) of Li[Al(OC$_{10}$F$_{15}$)$_4$]·2Et$_2$O.

NMR study of $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$ in D_2O, but the salt is hardly soluble in D_2O:

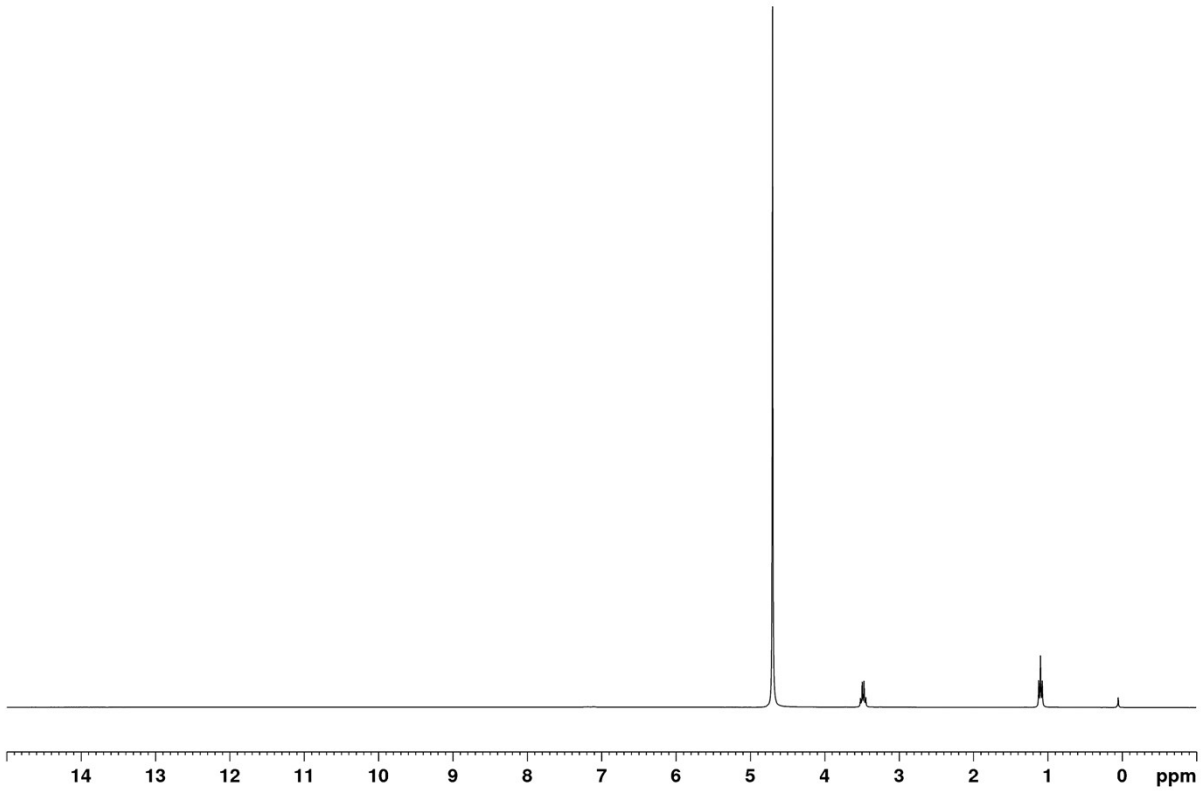


Figure S- 94: ^{1}H-NMR (300.18 MHz, 298 K, D_2O) H_2O stability of $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$.

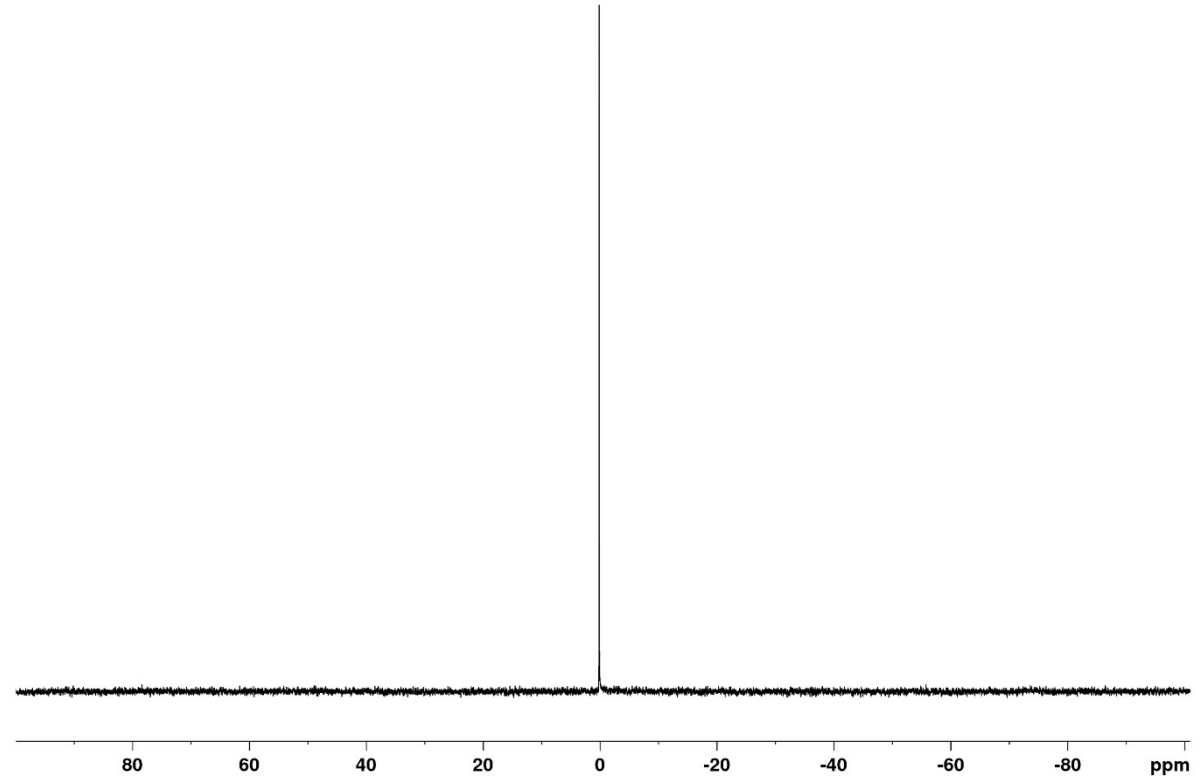


Figure S- 95: ^{7}Li-NMR (116.66 MHz, 298 K, D_2O) H_2O stability of $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$.

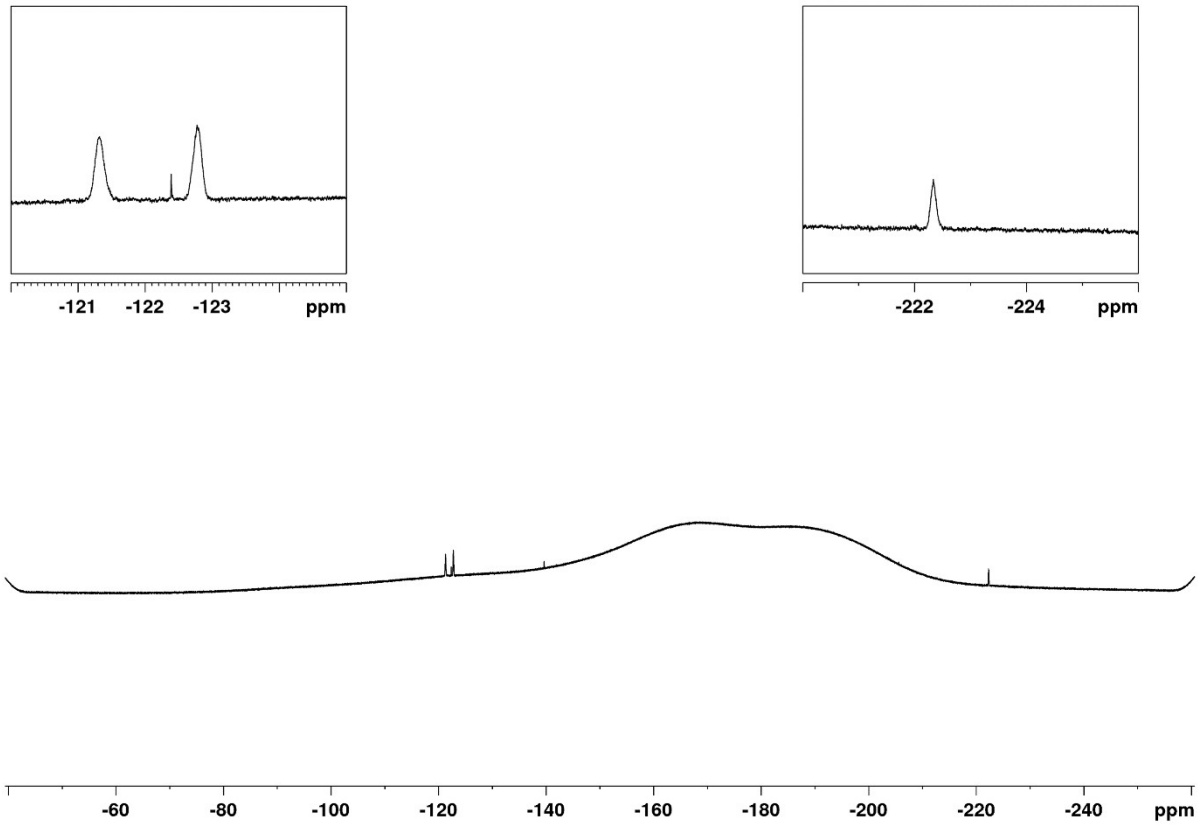


Figure S- 96: ^{19}F-NMR (282.45 MHz, 298 K, D_2O) H_2O stability of $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$.

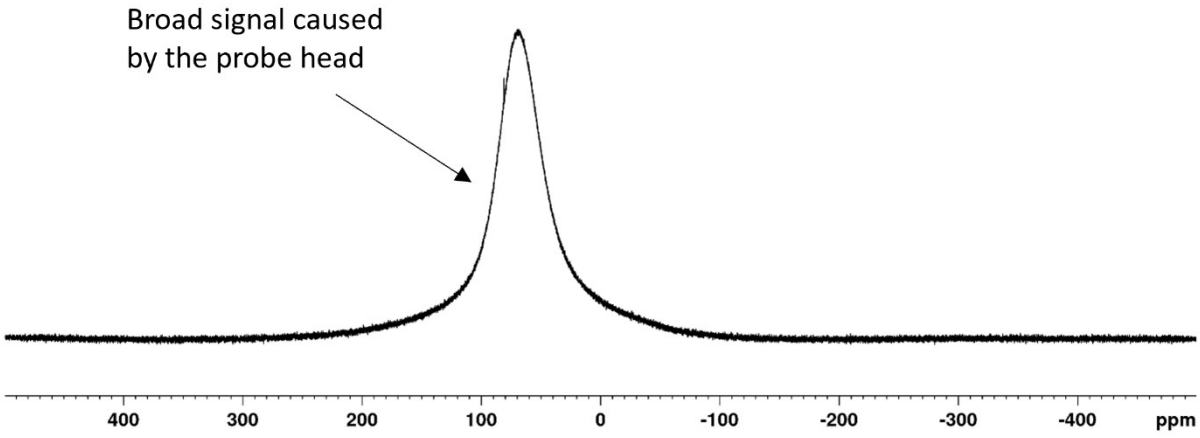


Figure S- 97: ^{27}Al-NMR (78.22 MHz, 298 K, D_2O) H_2O stability of $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$.

Synthesis of $[NO][Al(OC_{10}F_{15})_4]$ starting from pure $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$

$Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$ (0.243 g, 0.136 mmol) and $[NO][BF_4]$ (0.020 g, 0.171 mmol, 1.26 eq) were suspended in SO_2 (5.0 mL) and stirred for 5 days at r.t. The reaction mixture was filtered, and the solid residue extracted twice with SO_2. The solvent was removed under reduced pressure, the solid residue was washed with C_6F_6 (3x 1.0 mL) and dried under reduced pressure. The target compound was obtained as orange/brown solid (0.124 g, 0.071 mmol, 53 %) and analyzed by NMR spectroscopy.

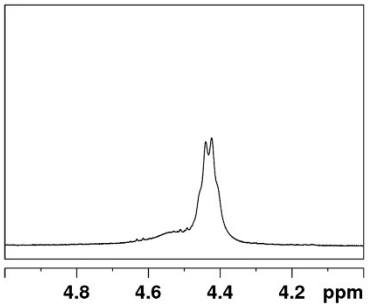
^{1}H-NMR (400.17 MHz, 298 K, SO_2): δ = 1.83 (t, 6H, C**H$_3$**CH$_2$OCH$_2$C**H$_3$**), 4.43 (q, 4H, CH$_3$C**H$_2$**OC**H$_2$**CH$_3$) ppm.

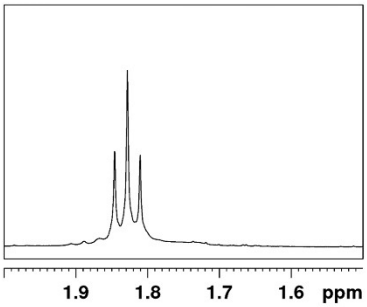
^{7}Li-NMR (155.52 MHz, 298 K, SO_2): no signal (as expected)

^{14}N-NMR (28.91 MHz, 298 K, SO_2): no signal

^{19}F-NMR (376.54 MHz, 298 K, SO_2): δ = −222.7 (m, C**F**, 12F, $[NO][Al(OC_{10}F_{15})_4]$), −163.0 (m, 6F, C_6F_6), −121.3 (m, C**F$_2$**, $[NO][Al(OC_{10}F_{15})_4]$), −120.9 (m, C**F$_2$**, $[NO][Al(OC_{10}F_{15})_4]$) ppm.

^{27}Al-NMR (104.27 MHz, 298 K, SO_2): δ = 35.1 (s, 1Al, $[NO][$**Al**$(OC_{10}F_{15})_4]$) ppm.





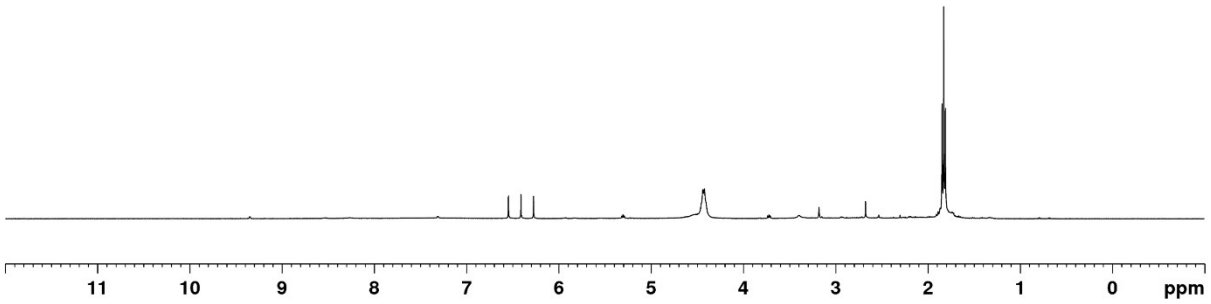


Figure S- 98: ^{1}H-NMR (400.17 MHz, 298 K, SO_2) Synthesis of $[NO][Al(OC_{10}F_{15})_4]$ starting from pure $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$.

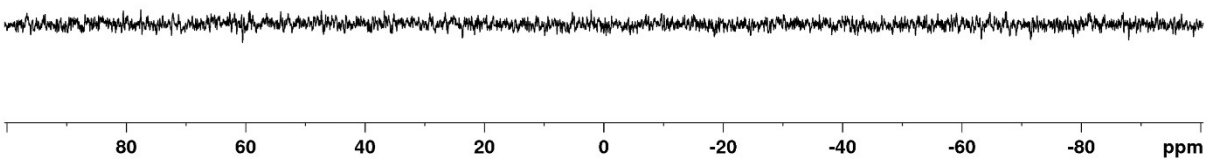


Figure S- 99: ^{7}Li-NMR (155.52 MHz, 298 K, SO_2) Synthesis of $[NO][Al(OC_{10}F_{15})_4]$ starting from pure $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$.

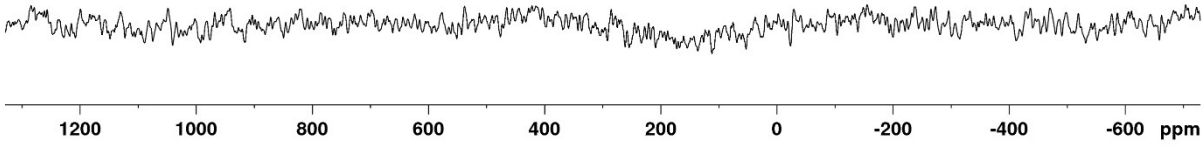


Figure S- 100: ^{14}N-NMR (28.91 MHz, 298 K, SO_2) Synthesis of [NO][Al($OC_{10}F_{15}$)$_4$] starting from pure Li[Al($OC_{10}F_{15}$)$_4$]·2Et_2O.

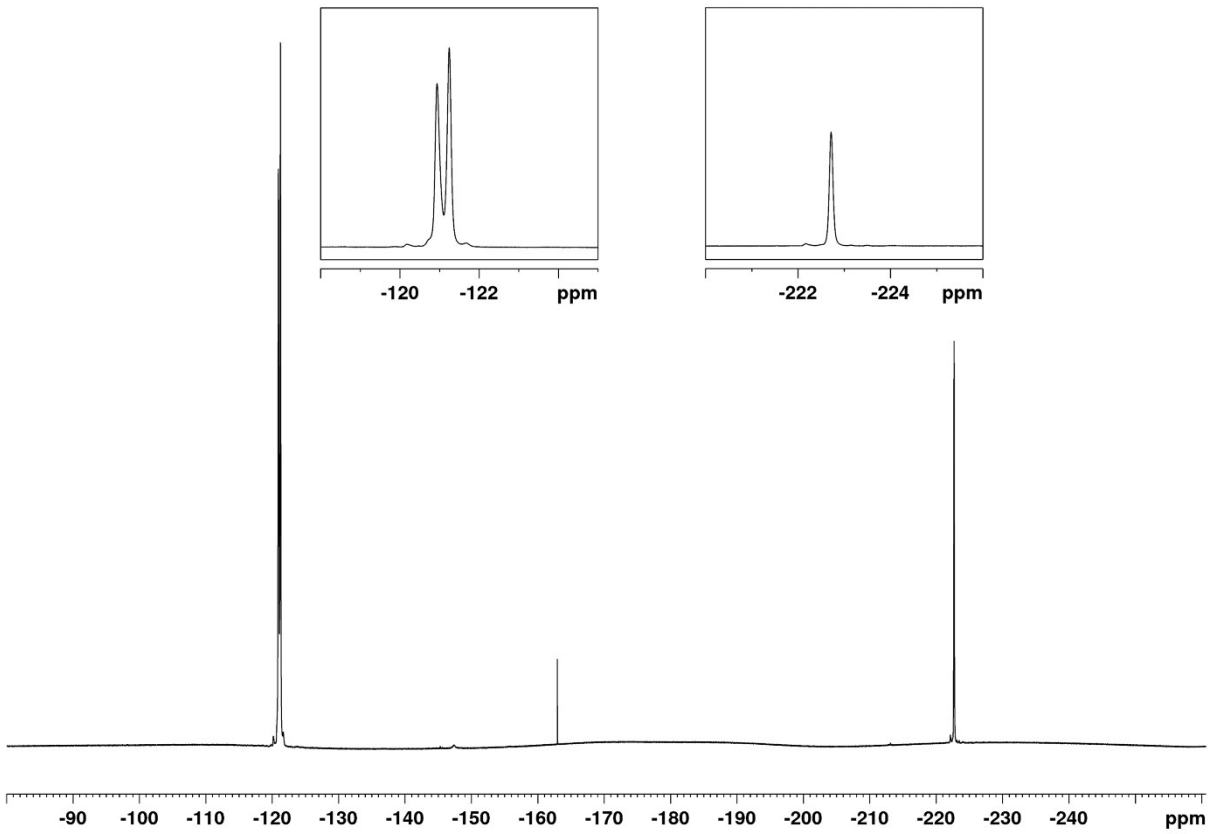


Figure S- 101: ^{19}F-NMR (376.54 MHz, 298 K, SO_2) Synthesis of [NO][Al($OC_{10}F_{15}$)$_4$] starting from pure Li[Al($OC_{10}F_{15}$)$_4$]·2Et_2O.

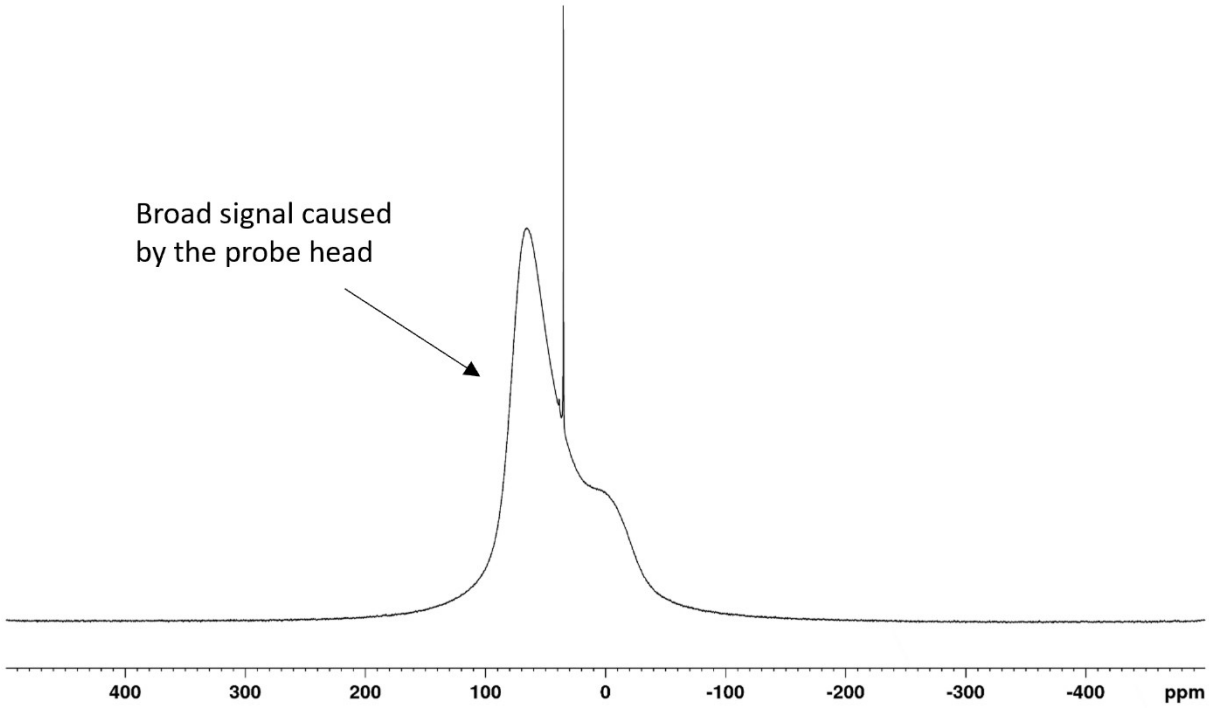


Figure S- 102: ^{27}Al-NMR (104.27 MHz, 298 K, SO_2) Synthesis of $[NO][Al(OC_{10}F_{15})_4]$ starting from pure $Li[Al(OC_{10}F_{15})_4]\cdot 2Et_2O$.

IR Spectroscopic Data of *Cat.*[*pfAd*]

Table S- 1: Overview of measured IR frequencies of pure salts of the [*pfAd*]$^-$ anion in comparison with the calculated vibrational frequencies of the [*pfAd*]$^-$ anion (BP86(D3BJ)/def-SV(P)). The assignment of the anion vibrations is based on the simulated IR spectrum of the anion. Here the intensities are given as: ≥ 0.8 = very strong (vs), ≥ 0.6 = strong (s), ≥ 0.4 = medium (m), ≥ 0.2 = weak (w), < 0.2 = very weak (vw).

$Ag(CH_2Cl_2)_2$[*pfAd*]	$[Ph_3C]$[*pfAd*]	Tl[*pfAd*]	$[H(OEt_2)_2]$[*pfAd*]	Calc. [*pfAd*]$^-$	Assignment
402 (vw)	402 (vw)	402 (w)	402 (w)	397 (vw)	δ(O−Al−O)
442 (vw)	441 (vw)	441 (m)	443 (w)	434 (vw)	ν(C−C), δ(O−Al−O)
	467 (vw)				
533 (vw)	533 (vw)	533 (vw)	533 (vw)	525 (vw)	ν(C−C), δ(O−Al−O), ν(C−F)
	609 (vw)				
	624 (vw)				
		643 (vw)			
651 (vw)	650 (vw)	651 (w)	652 (w)	635 (vw)	ν(C−F), ν(C−C)
679 (vw)	678 (vw)	678 (w)	679 (vw)	667 (vw)	ν(Al−O), ν(C−C), ν(C−F)
	704 (vw)				
736 (vw)					
758 (vw)	756 (vw)	762 (vw)	760 (vw)	756 (vw)	ν(Al−O)
	767 (vw)				
	807 (vw)				
814 (vw)					
	843 (vw)				
852 (vw)					
			905 (w)		
955 (vs)	955 (vs)	954 (vs)	955 (vs)	961 (s)	ν(C−C)
981 (m)	978 (m)	979 (s)	981 (m)	972 (m)	ν(C−C), ν(C−F)
			1016 (vw)		
1038 (vw)					
1106 (vw)	1105 (vw)	1109 (vw)	1108 (vw)	1095 (vw)	ν(Al−O), ν(C−C)
	1189 (vw)		1192 (vw)	1209 (vw)	ν(C−C)
			1255 (m)		
1268 (vs)	1269 (vs)	1268 (vs)	1269 (vs)	1250 (vs)	ν(C−C)
	1293 (w)	1292 (w)	1295 (vw)	1280 (w)	ν(C−C)
1351 (vw)	1360 (w)	1350 (vw)	1353 (vw)	1363 (w)	ν(Al−O), ν(C−O)
			1392 (vw)		
	1454 (vw)				
	1486 (vw)				
	1585 (w)				
		1686 (vw)			
		1697 (vw)			
2966 (vw)					

Single-Crystal XRD Data

Table S- 2: Crystallographic data for complexes 2-*o*DFB, 3, 4 and 7.

	2-*o*DFB	**3**	**4**	**7**
CCDC number	2224626	2224627	2224628	2224629
Empirical formula	$C_{52}H_8AgAlF_{64}O_4$	$C_{90}H_{20}Ag_3AlF_{100}O_6$	$C_{60}H_{17}AlCl_2F_{60}O_4$	$C_{48}H_{21}AlF_{60}O_6$
Formula weight	2047.42	3447.66	2039.62	1860.63
Temperature [K]	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	orthorhombic	monoclinic	monoclinic
Space group (number)	$P2_1/n$ (14)	$P2_12_12_1$ (19)	$P2_1/n$ (14)	$P2_1/n$ (14)
***a* [Å]**	16.213(9)	14.9498(7)	12.724(9)	18.440(4)
***b* [Å]**	21.156(11)	18.4428(12)	22.259(17)	14.863(4)
***c* [Å]**	17.210(6)	36.6960(19)	23.784(18)	22.062(5)
α [°]	90	90	90	90
β [°]	91.208(6)	90	101.54(2)	104.402(9)
γ [°]	90	90	90	90
Volume [Å^3]	5902(5)	10117.7(10)	6600(8)	5857(3)
Z	4	4	4	4
ρ_{calc} [gcm^{-3}]	2.304	2.263	2.053	2.110
μ [mm^{-1}]	0.611	0.826	0.334	0.279
***F*(000)**	3952	6648	3984	3640
Crystal size [mm^3]	0.240×0.140×0.080	0.300×0.150×0.070	0.350×0.200×0.200	0.277×0.204×0.088
Crystal color	colorless	colorless	yellow	colorless
Crystal shape	block	needle	block	plate
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2θ range [°]	3.05 to 55.86 (0.76 Å)	2.22 to 57.42 (0.74 Å)	2.53 to 63.08 (0.68 Å)	3.32 to 54.25 (0.78 Å)
Index ranges	−21 ≤ h ≤ 21 −27 ≤ k ≤ 27 −22 ≤ l ≤ 22	−20 ≤ h ≤ 18 −23 ≤ k ≤ 24 −49 ≤ l ≤ 46	−18 ≤ h ≤ 18 −32 ≤ k ≤ 32 −34 ≤ l ≤ 34	−23 ≤ h ≤ 23 −19 ≤ k ≤ 19 −28 ≤ l ≤ 27
Reflections collected	225524	91049	240992	119781
Independent reflections	14129 R_{int} = 0.0579 R_{sigma} = 0.0273	25175 R_{int} = 0.0293 R_{sigma} = 0.0375	21931 R_{int} = 0.0410 R_{sigma} = 0.0217	12932 R_{int} = 0.0561 R_{sigma} = 0.0301
Completeness to θ = 25.242°	100.0 %	100.0 %	100.0 %	100.0 %
Data / Restraints / Parameters	14129/20713/1971	25175/68351/3609	21931/83/1172	12932/198/1091
Goodness-of-fit on F^2	1.105	1.078	1.048	1.101
Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0517 wR_2 = 0.1227	R_1 = 0.0402 wR_2 = 0.0782	R_1 = 0.0458 wR_2 = 0.1143	R_1 = 0.0614 wR_2 = 0.1269
Final *R* indexes [all data]	R_1 = 0.0800 wR_2 = 0.1383	R_1 = 0.0499 wR_2 = 0.0822	R_1 = 0.0655 wR_2 = 0.1270	R_1 = 0.0866 wR_2 = 0.1387
Largest peak/hole [eÅ^{-3}]	0.87/-0.87	0.71/-0.62	0.81/-0.62	0.44/-0.44

Single-Crystal XRD Data – Discussion

[Ag(o-DFB)$_2$][Al(OC$_{10}$F$_{15}$)$_4$] (**2-*o*DFB**):

Crystals of *[Ag(o-DFB)$_2$][Al(OC$_{10}$F$_{15}$)$_4$]* (**2-*o*DFB**) were obtained as colorless blocks by gas phase diffusion of *n*-pentane into a solution of Ag[*pfAd*] in *o*-DFB. The structure is strongly disordered, and thus a discussion of the structural parameters of the [Al(OC$_{10}$F$_{15}$)$_4$]$^-$ anion is prohibited.

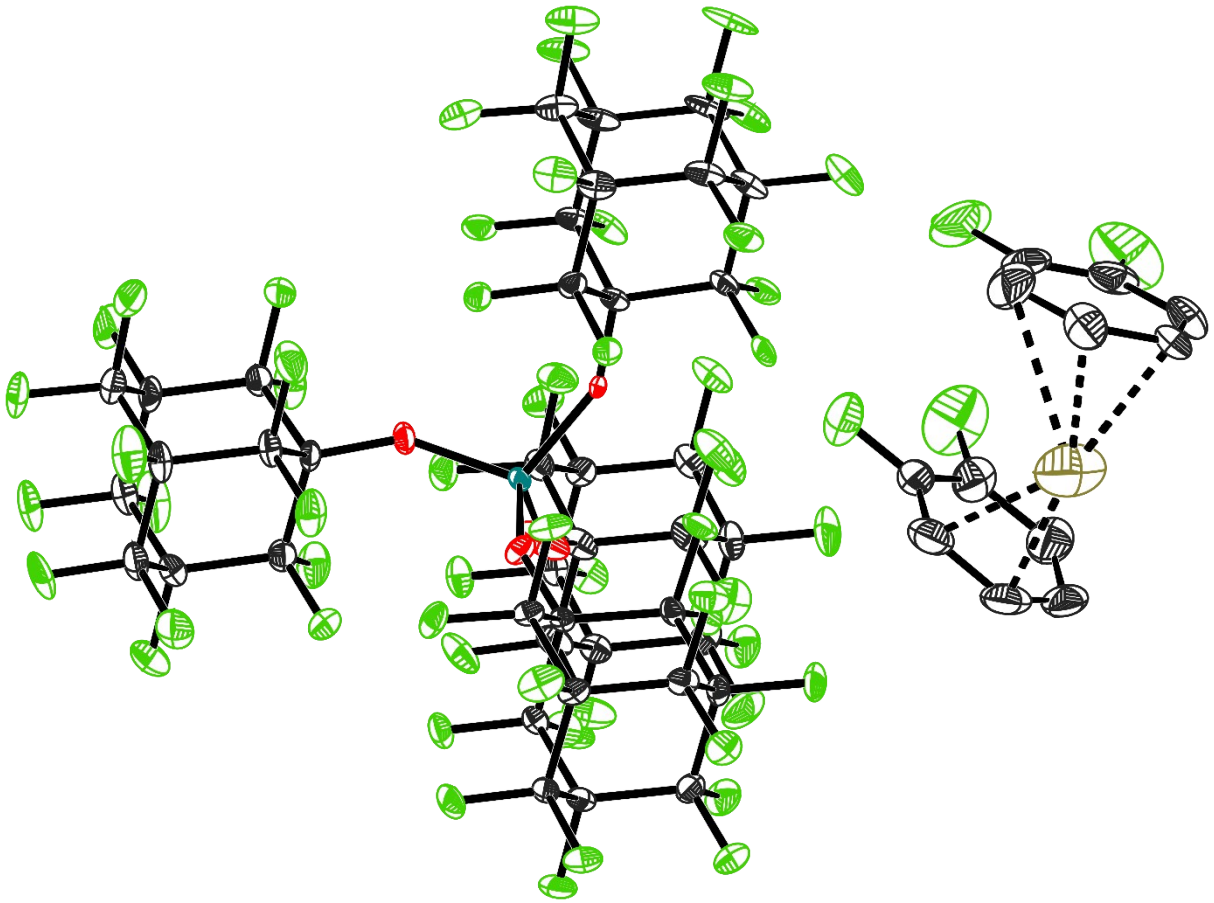


Figure S-103: Molecular structure of *Ag[Al(OC$_{10}$F$_{15}$)$_4$] (2-oDFB)with thermal ellipsoids set at 50 % probability level. The structure is disordered, and* for clarity, only the main PARTs are shown. Scheme: Al (turquoise), O (red), F (green), C (black), Ag (yellow-brown), hydrogen atoms omitted for clarity.

[Ag$_3$(OC$_{10}$F$_{15}$)$_2$(o-DFB)$_3$][Al(OC$_{10}$F$_{15}$)$_4$] (**3**):

Colorless needles of [Ag$_3$(OC$_{10}$F$_{15}$)$_2$(*o*-DFB)$_3$][Al(OC$_{10}$F$_{15}$)$_4$] (**3**) were obtained by gas phase diffusion of *n*-pentane into solution of Ag[*pfAd*] in *o*-DFB (containing AgOC$_{10}$F$_{15}$ impurities).

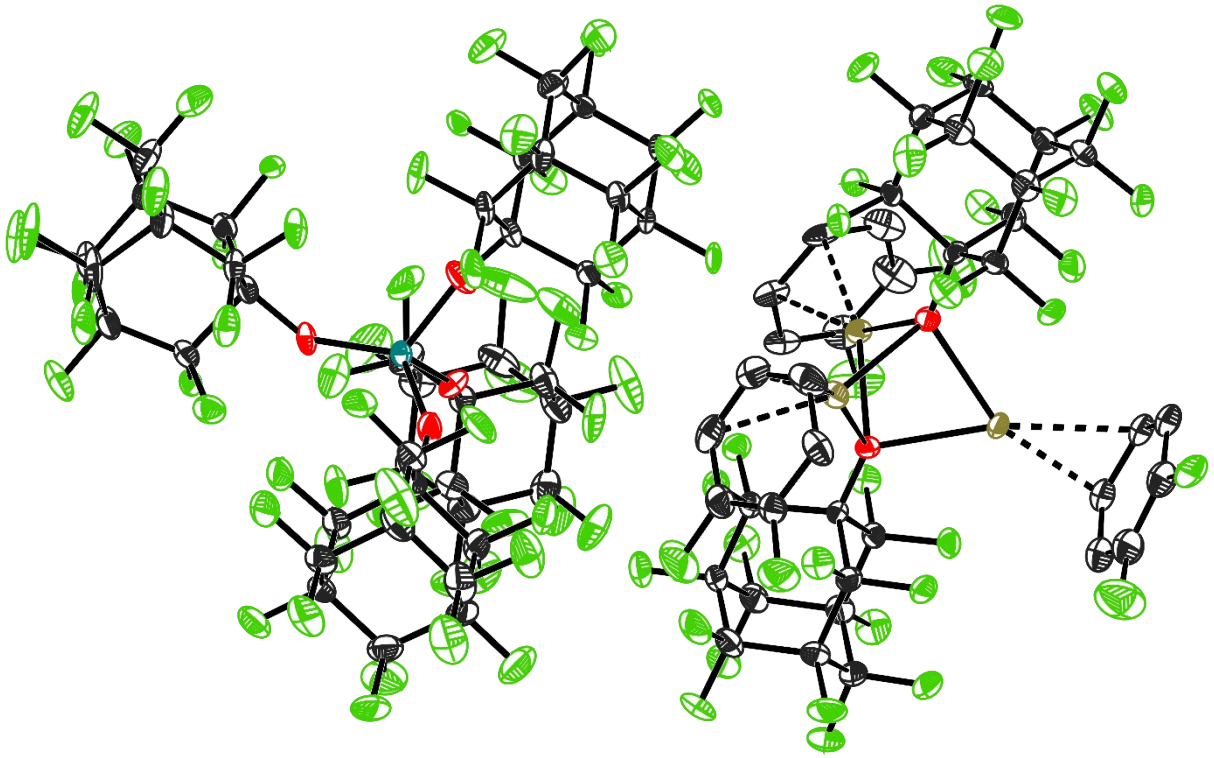


Figure S- 104: Molecular structure of *[Ag$_3$(OC$_{10}$F$_{15}$)$_2$(o-DFB)$_3$][Al(OC$_{10}$F$_{15}$)$_4$] (3) with thermal ellipsoids set at 50 % probability level. The structure is heavily disordered, and* for clarity, only the main PARTs are shown. Scheme: Al (turquoise), O (red), F (green), C (black), Ag (yellow-brown), hydrogen atoms omitted for clarity.

The cation in **3** can be described as a trigonal bipyramidal cluster formed by three silver atoms, which span a nearly equilateral triangle, and two perfluoro-adamantanoxy residues, each being coordinated to the three silver atoms via the oxygen atom. Interestingly, the OC$_{10}$F$_{15}$ residues are the only positions within the molecular structure, which are not disordered. The disorder of the [*pfAd*]$^-$ anion is shown in Figure S- 105. Each silver atom is further coordinated by an *o*-DFB molecule, which is bound via its carbon atom(s) in a η^2- or η^3-fashion. Two of the silver atoms are additionally coordinated by another *o*-DFB molecule via one of the fluorine atoms. An occupation number of 4 % for these silver atoms indicates only a weak interaction, Figure S- 106. Consequently, this interaction was omitted in the main part discussion. Such trigonal bipyramidal structural motif of group 10 or 11 metal clusters is well known. Usually, these structures are capped by μ^3 ligands and carry bridging, bidentate *bis*(diphenylphosphino)methane (dppm) or *bis*(diphenylphosphino)ethane (dppe) ligands.[21,22] Structures without the chelating phosphine ligands, however, were unknown until 2007.[22] The reaction of Ag[*pf*] with 2 eq. of AgOC(CF$_3$)$_3$ in CH$_2$Cl$_2$ allows the formation of [(Ag(OR^F)$_2$(L)$_3$][pf], and the presence of soft donor molecules L such as C$_2$H$_4$ or *i*-C$_4$H$_8$ is crucial for the synthesis of the trigonal bipyramidal cation. The Ag–Ag interactions are supposed to be very weak, and consequently, the trinuclear silver cluster can be regarded as an aggregate of three [Ag(L)]$^+$ cations and two OR^F anions (with OR^F = OC(CF$_3$)$_3$, OC$_{10}$F$_{15}$), held together mainly by electrostatic interactions.[22] The observation of [Ag$_3$(OC$_{10}$F$_{15}$)$_2$(*o*-DFB)$_3$][Al(OC$_{10}$F$_{15}$)$_4$] is a further, so far unknown example of a group 11 metal structure showing the trigonal bipyramidal framework, stabilized by *o*-DFB.

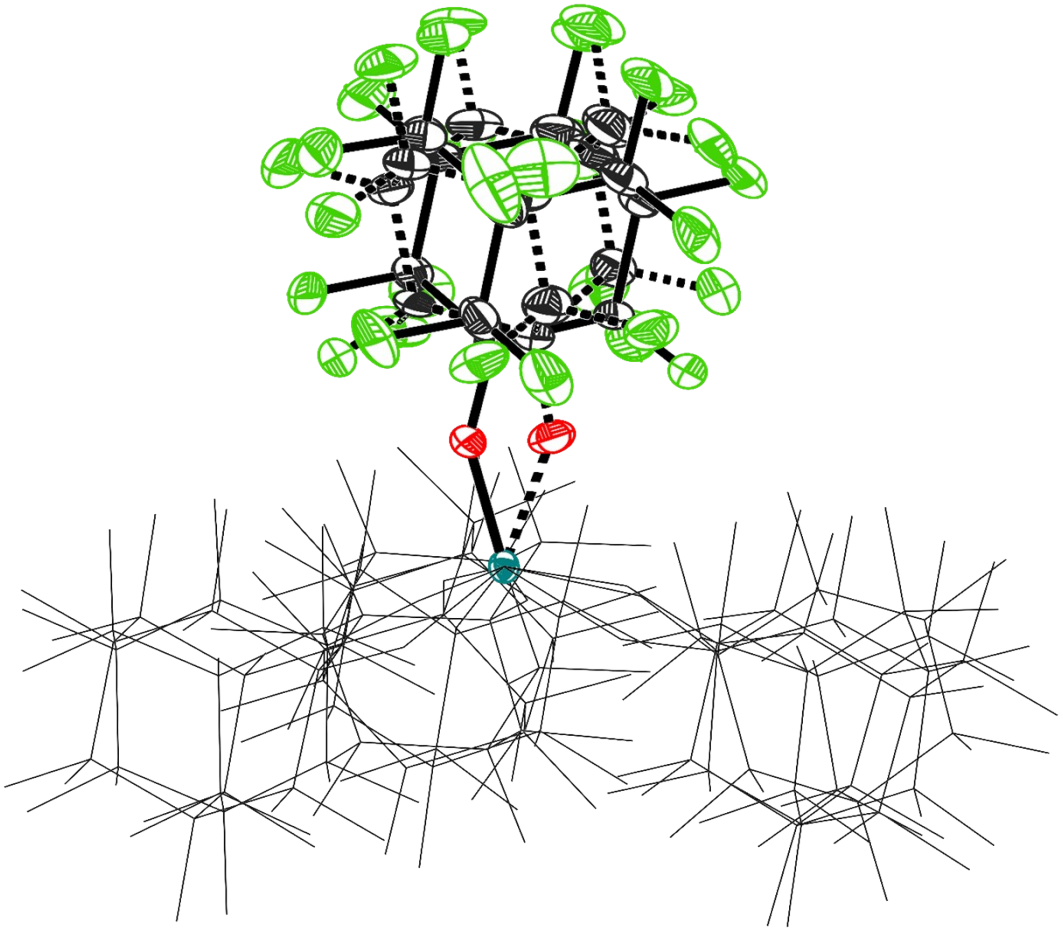


Figure S- 105: Illustration of the [*pfAd*]$^-$ anion disorder. In contrast to the [*pf*]$^-$ anion where CF_3 groups tend to rotate, the alkoxy residues in the [*pfAd*]$^-$ anion tend to rotate/switch between positions in total.

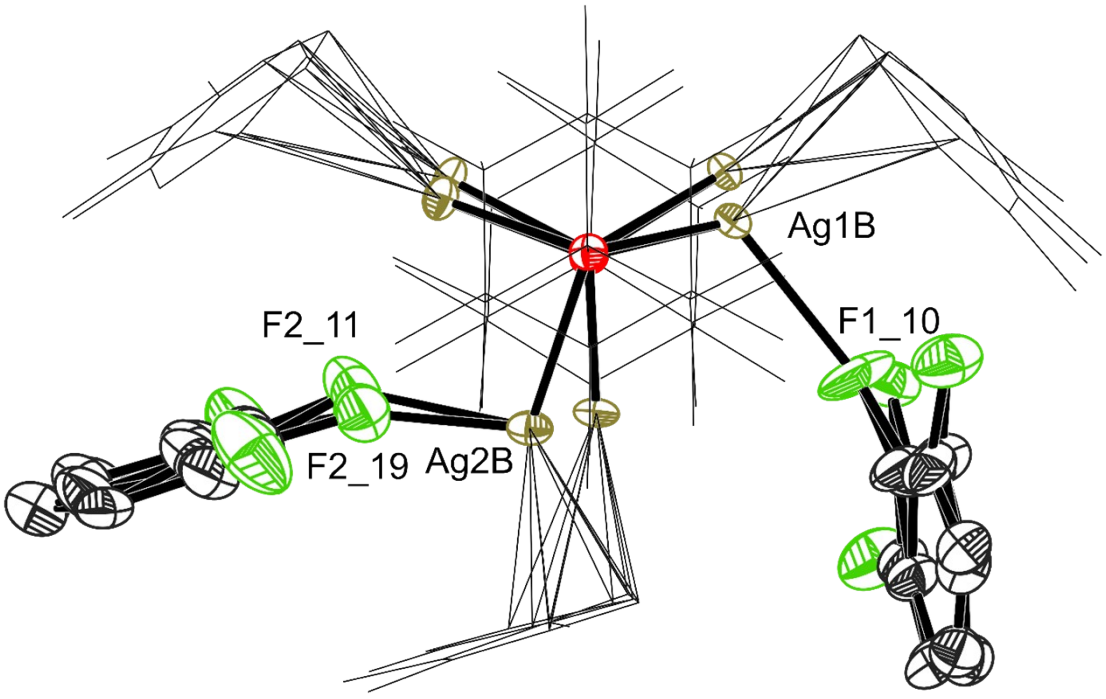


Figure S- 106: Illustration of the additional *o*-DFB coordination towards two Ag^+ with occupation numbers of only 4 %. The highlighted distances amount to Ag1B-F1_10 2.42(2) Å, Ag2B-F2_19 2.09(4) Å and Ag2B-F2_11 2.25(3) Å. Since the occupation number of this part is only 4 %, this coordination was not shown in the main part for clarity.

[Ph$_3$C][Al(OC$_{10}$F$_{15}$)$_4$] (**4**):

Crystals of [Ph$_3$C][Al(OC$_{10}$F$_{15}$)$_4$] (**4**) suitable for scXRD analysis were obtained as yellow blocks by gas phase diffusion of *n*-pentane into a solution of **4** in CH_2Cl_2.

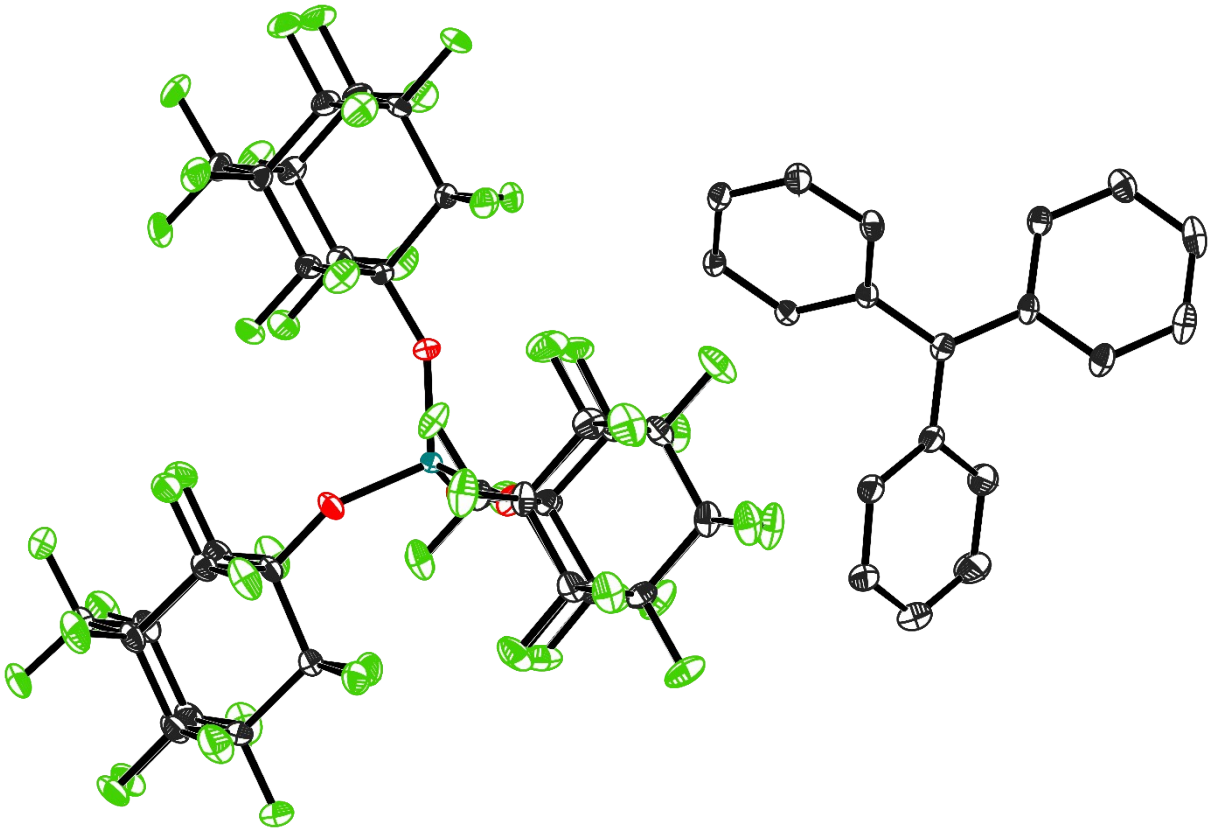


Figure S- 107: Molecular structure of *[Ph$_3$C][Al(OC$_{10}$F$_{15}$)$_4$] (4) with thermal ellipsoids set at 50 % probability level.* Scheme: Al (turquoise), O (red), F (green), C (black), hydrogen atoms omitted for clarity.

Tl[Al(OC$_{10}$F$_{15}$)$_4$] (**6**)*:*

Crystals of Tl[Al(OC$_{10}$F$_{15}$)$_4$] (**6**) were obtained by gas phase diffusion of *n*-pentane into a solution of Tl[Al(OC$_{10}$F$_{15}$)$_4$] (**6**) in *o*-DFB. While the crystals were suitable for scXRD analysis and the reflection data were of good quality, a satisfying model could not be obtained. We would nevertheless like to describe what we know about the structure.

An initial analysis resulted in the space group R-3, and the position both, of the anion and of the Tl^+ cation could (seemingly) be located (Tl atoms(s) in the middle of Figure S- 108). This thallium atom appears to be surrounded by two [*pfAd*]$^-$ anions and thus by six perfluoro-adamantanolate units. It is located near to one of the threefold rotoinversion centers of the cell. However, quite a substantial amount of residual density of ca. 19 e/Å^3 remained undescribed. A description by another Tl atom (Tl atoms in the right of Figure S- 108; connected to the first one by a free variable) solved this issue. However, upon filling the cell, a substantial void remained, which could perfectly host another perfluoro-adamantanolate fragment. Further, the symmetry elements of the space group cause the second Tl atom to surround this void in a trigonal prismatic fashion. Obviously, another threefold rotoinversion center is located in the middle of this void. However, we did not manage to model a reasonable description of the void. While we modelled the disorder of one of the perfluoro-

adamantolate ligands of the main [*pfAd*]$^-$ anion by a threefold disorder with all three PARTs being bound to the same aluminum atom, we believe that the disorder is rather described by another orientation of one of the perfluoro-adamantolate moieties, and we believe that this PART is bound to the perfluoro-adamantanolate in the void. This subtlety, however, cannot be resolved due to the very similar electron density of oxygen and fluorine. Further, we could not locate the additional aluminum atom, which would be necessary for this description.

In sum, the structure is mainly determined by a close packing of the perfluoro-adamantolate units (with different orientations and not with the same occupation) in which thallium atoms are embedded at two crystallographically different positions. We do not believe any co-crystallization of solvent molecules (also based on the NMR-spectroscopic investigation of the crystals). However, we are not able to provide a satisfying model. As a Supporting Information, we attached the cif file (including structure factors) from which the illustration given in Figure S- 108 was generated.

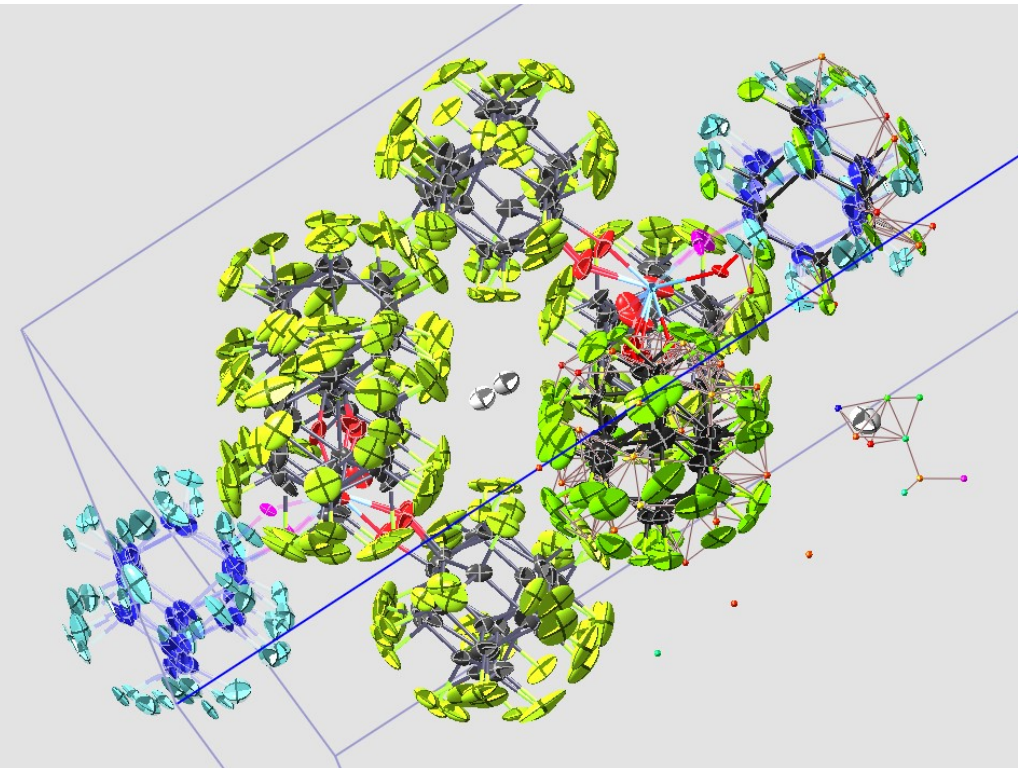


Figure S- 108: Illustration of the incomplete model for the description of the molecular structure of $Tl[Al(OC_{10}F_{15})_4]$. The figure clarifies and visualizes the mentioned issues which prevent obtaining a satisfying solution.

[H(OEt$_2$)$_2$][Al(OC$_{10}$F$_{15}$)$_4$] (**7**):

Crystals suitable for scXRD analysis were obtained by storage of a solution of [H(OEt$_2$)$_2$][*pfAd*] (**7**) in *o*-DFB at −40 °C.

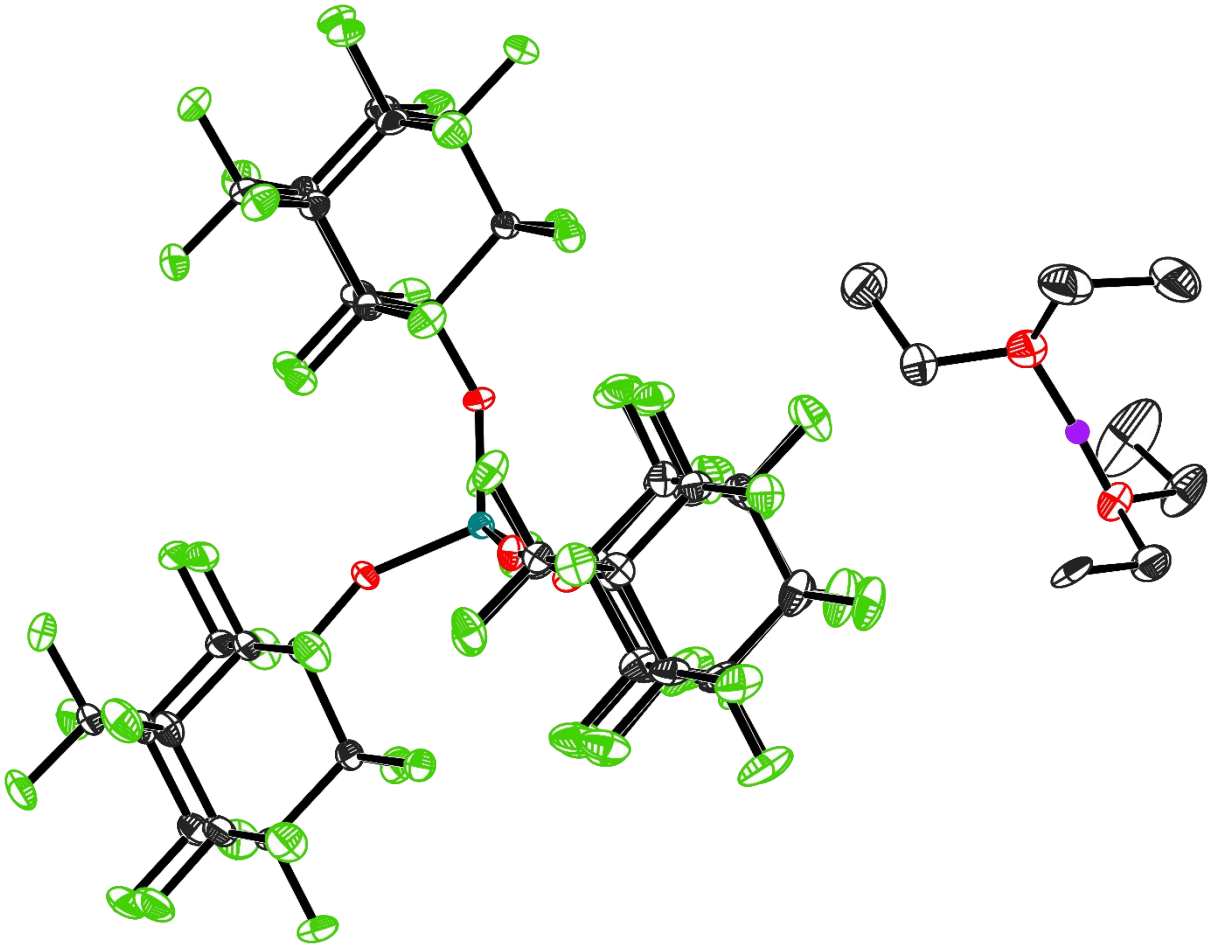


Figure S- 109: Molecular structure of *[H(OEt$_2$)$_2$][Al(OC$_{10}$F$_{15}$)$_4$] (7) with thermal ellipsoids set at 50 % probability level.* Scheme: Al (turquoise), O (red), F (green), C (black), hydrogen atoms omitted for clarity except the acidic, bridging proton (purple).

The [H(OEt$_2$)$_2$]$^+$ cation within the molecular structure is disordered. While one of the ether moieties has a fixed position, the one located nearer to the anion is described by two parts (occupations of 0.644 and 0.356). Overall, the general description of the binding situation is very similar to that within [H(OEt$_2$)$_2$][Al(OC(CF$_3$)$_3$)$_4$].[23] Since the position of the proton is difficult to deduce, the evaluation of the O–O distance is more reliable. In **7**, the O–O distance amounts to 245.1(12) pm (for the major PART) and 235(2) pm (for the minor PART). In [H(OEt$_2$)$_2$][*pf*], this distance amounts to 242.4 pm, and in other [H(OEt$_2$)$_2$]$^+$ salts, the values range between 240 to 245 pm.[23,24] Obviously, the O–O distance of 235(2) pm (for the minor PART) is particularly small, which might be attributed to a particularly weak interaction with the anion. Indeed, the disordered ether molecule with the higher occupation (and the longer O–O distance) exhibits slight H–F interactions, while the ether molecule with the lower occupation (and the shorter O–O distance) does not show any contacts to the anion.

Quantum Chemical Calculations

Fluoride Ion Affinity (FIA)

The fluoride ion affinity was calculated with TURBOMOLE as followed by the use of the reaction enthalpy of 952.5 kJ mol^{-1} for equation two, the reaction of Me_3Si^+ with F^- to Me_3SiF, as benchmark which was calculated by the group of *L. Greb*.[25] For a detailed description how to calculate the FIA, the reader is referred to the already mentioned paper of *P. Erdmann et al*.[25]

$$A + Me_3Si\text{-}F \xrightarrow[BP86/SV(P)]{\text{isodesmic}} A\text{-}F^- + Me_3Si^+$$

$$Me_3Si^+ + F^- \xrightarrow{\Delta H_{calc.} = -952.5\ \text{kJ mol}^{-1}} Me_3Si\text{-}F$$

$$A + F^- \xrightarrow{-\Delta H = \text{FIA}} A\text{-}F^-$$

Scheme S- 1: Underlying reactions for calculating the fluoride ion affinity FIA.

Table S- 3: Summary of thermodynamic data calculated at the BP86(D3BJ)/def-SV(P) level of theory (grid m3, 298.15 K) for the calculation of the FIA:

	E_{SCF} / H	E_{SCF} / kJ·mol^{-1}	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	$G°$ / kJ·mol^{-1}	$H°$ / kJ·mol^{-1}
Me_3SiF	-508.94	-1336232.32	311.17	0.35193	-1336023.60	-1335918.67
Me_3Si^+	-408.82	-1073364.34	297.88	0.35707	-1073170.45	-1073063.98
$B(OCH(CF_3)_2)_3$	-2391.01	-6277606.11	497.71	0.88587	-6277370.04	-6277105.92
$[FB(OCH(CF_3)_2)_3]^-$	-2490.92	-6539915.93	501.08	0.87361	-6539672.83	-6539412.37
$B(C_6F_5)_3$	-2206.83	-5794041.26	472.69	0.81730	-5793809.77	-5793566.09
$[FB(C_6F_5)_3]^-$	-2306.76	-6056398.19	478.69	0.84713	-6056169.59	-6055917.02
$Ga(C_2F_5)_3$	-3649.97	-9582982.68	260.03	0.72732	-9582937.02	-9582720.17
$[FGa(C_2F_5)_3]^-$	-3749.90	-9845371.25	267.45	0.73042	-9845319.09	-9845101.32
$B(OC_5F_4N)_3$	-2183.11	-5731765.27	482.91	0.84514	-5731531.86	-5731279.88
$[FB(OC_5F_4N)_3]^-$	-2283.06	-5994166.87	488.00	0.83021	-5993923.92	-5993676.39
$Al(OC(CF_3)_3)_3$	-3619.01	-9501700.91	541.91	1.05638	-9501471.48	-9501156.52
$[FAl(OC(CF_3)_3)_3]^-$	-3718.97	-9764146.57	550.66	1.11408	-9763925.60	-9763593.44
$Al(C_6F_5)_3$	-2424.39	-6365246.54	463.17	0.87140	-6365040.69	-6364780.89
$[FAl(C_6F_5)_3]^-$	-2524.36	-6627694.26	469.38	0.89970	-6627490.65	-6627222.40
$Al(OTeF_5)_3$	-1988.88	-5221794.53	199.43	0.79318	-5221829.11	-5221592.62
$[FAl(OTeF_5)_3]^-$	-2088.84	-5484251.88	209.76	0.86464	-5484297.44	-5484039.64
$Ga(OTeF_5)_3$	-3671.29	-9638964.99	197.06	0.81575	-9639008.66	-9638765.45
$[FGa(OTeF_5)_3]^-$	-3771.25	-9901422.08	206.56	0.88166	-9901475.91	-9901213.04

$Al(OC_5F_4N)_3$	-2400.71	-6303057.10	470.46	0.81449	-6302827.00	-6302584.16
$[FAl(OC_5F_4N)_3]^-$	-2500.69	-6565550.75	480.82	0.85687	-6565322.93	-6565067.45
$Al(OC_{10}F_{15})_3$	-6100.25	-16016196.81	1042.73	1.42939	-16015577.77	-16015151.60
$[FAl(OC_{10}F_{15})_3]^-$	-6200.23	-16278692.06	1051.05	1.47869	-16278079.40	-16277638.53

Standard enthalpy *H°* and Gibbs energy *G°* were calculated according to equation S1 and S2 at 298.15 K and 0.1 MPa:

$$H^0 = E_{SCF} + E_{vrt} + RT \quad (1)$$

$$G^0 = H^0 - T \cdot S^0 \quad (2)$$

Where E_{SCF} is the electronic energy, E_{vrt} is the sum of translational, rotational, and vibrational energy inclusive zero-point energy, *S°* is the standard entropy, *R* ideal gas constant and *T* is the temperature in Kelvin.

To obtain a more reliable and comparable (e.g. with the recently published FIA paper of *L. Greb*[25]) FIA value for the novel $[pfAd]^-$ anion, the geometry of the structures TMSF, TMS^+, $Al(OC_{10}F_{15})_3$ and $[FAl(OC_{10}F_{15})_3]^-$ were additionally optimized on pbeh-3c[26]/def2-mSVP[26] level of theory with TURBOMOLE and afterwards single point calculations were performed on DLPNO-CCSD(T)[27]/cc-pVQZ[28] with RIJCOSX level of theory using ORCA[29] (v4.2.1, normal PNO and tight SCF thresholds) to obtain more reliable E_{SCF} values.

Table S- 4: Summary of thermodynamic data calculated at the DLPNO-CCSD(T)/cc-VPQZ//pbeh-3c/def2-mSVP level of theory (grid m4, 298.15 K) for the calculation of the FIA of the $[pfAd]^-$:

	E_{SCF} / H	E_{SCF} / kJ·mol^{-1}	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	$G°$ / kJ·mol^{-1}	$H°$ / kJ·mol^{-1}
Me_3SiF	-508.50	-1335065.43	328.91	0.34934	-1334838.20	-1334734.04
Me_3Si^+	-408.36	-1072154.63	315.02	0.35410	-1071942.71	-1071837.13
$Al(OC_{10}F_{15})_3$	-6098.45	-16011486.88	1099.09	1.39491	-16010801.21	-16010385.31
$[FAl(OC_{10}F_{15})_3]^-$	-6198.45	-16274035.45	1106.88	1.44958	-16273358.28	-16272926.09

For future calculations and comparisons, the thermodynamic values (FIA, LA, PD, CuD) were additionally calculated at the more reliable DSD-PBEP86(D3BJ)[30]/def2-QZVPP[31]//pbeh-3c[26]/def2-mSVP[26] level of theory using ORCA (v5.0.2) with RIJCOSX for the single point calculation, Table S- 5. **Note:** Detailed results for the structures calculated on this level of theory are not listed here, just all the obtained thermodynamic values which are needed for calculating the FIA, LA, PD and CuD.

Table S- 5: Summary of thermodynamic data calculated at the DSD-PBEP86(D3BJ)/def2-QZVPP//pbeh-3c/def2-mSVP level of theory (298.15 K) for the calculation of the FIA, LA, PD and CuD:

	E_{SCF}(pbeh3-c) / H	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	E_{SCF}(PBEP86) / H	$H°$ (PBEP86)/ kJ·mol^{-1}
Me_3SiF	-508.37	328.91	0.34934	-508.69	-1335224.53
Me_3Si^+	-408.35	315.02	0.35367	-408.54	-1072315.43
$B(OCH(CF_3)_2)_3$	-2388.00	521.88	0.87283	-2390.77	-6276436.11
$[FB(OCH(CF_3)_2)_3]^-$	-2487.80	525.53	0.87196	-2490.69	-6538783.23

$[B(OCH(CF_3)_2)_4]^-$	-3175.82	684.67	1.04501	-3179.51	-8347127.91
$B(C_6F_5)_3$	-2203.92	496.84	0.78992	-2206.30	-5792154.24
$[FB(C_6F_5)_3]^-$	-2303.74	503.83	0.81184	-2306.25	-6054551.40
$[B(C_6F_5)_4]^-$	-2930.41	655.82	0.94235	-2933.60	-7701518.67
$Ga(C_2F_5)_3$	-3646.84	273.22	0.71374	-3649.15	-9580557.95
$[FGa(C_2F_5)_3]^-$	-3746.67	280.21	0.71952	-3749.11	-9843015.32
$[Ga(C_2F_5)_4]^-$	-4221.30	361.09	0.82082	-4224.29	-11090509.17
$B(OC_5F_4N)_3$	-2180.17	507.87	0.81250	-2182.54	-5730258.26
$[FB(OC_5F_4N)_3]^-$	-2280.00	513.33	0.79917	-2282.49	-5992685.05
$[B(OC_5F_4N)_4]^-$	-2898.75	668.13	0.97460	-2901.91	-7618968.68
$Al(OC(CF_3)_3)_3$	-3614.53	568.92	1.02499	-3618.52	-9499865.33
$[FAl(OC(CF_3)_3)_3]^-$	-3714.38	577.17	1.08744	-3718.51	-9762368.53
$[Al(OC(CF_3)_3)_4]^-$	-4738.79	755.93	1.30617	-4744.11	-12454903.89
$Al(C_6F_5)_3$	-2421.25	486.95	0.83739	-2423.69	-6362909.98
$[FAl(C_6F_5)_3]^-$	-2521.11	493.62	0.87845	-2523.68	-6625412.86
$[Al(C_6F_5)_4]^-$	-3147.76	645.01	1.01206	-3151.00	-8272306.61
$Al(OTeF_5)_3$	-2766.42	211.83	0.78957	-2767.94	-7267021.41
$[FAl(OTeF_5)_3]^-$	-2866.29	220.75	0.83607	-2867.95	-7529581.37
$[Al(OTeF_5)_4]^-$	-3608.00	280.6	1.01925	-3610.03	-9477838.24
$Ga(OTeF_5)_3$	-4448.10	209.12	0.81191	-4449.86	-11682893.56
$[FGa(OTeF_5)_3]^-$	-4547.96	217.86	0.84707	-4549.85	-11945420.94
$[Ga(OTeF_5)_4]^-$	-5289.68	277.73	1.01745	-5291.94	-13893695.98
$Al(OC_5F_4N)_3$	-2397.53	495.35	0.80033	-2399.96	-6301098.69
$[FAl(OC_5F_4N)_3]^-$	-2497.41	505.00	0.85926	-2499.96	-6563652.55
$[Al(OC_5F_4N)_4]^-$	-3116.16	659.52	1.06203	-3119.38	-8189930.15
$Al(OC_{10}F_{15})_3$	-6092.54	1099.09	1.39482	-6099.29	-16012580.72
$[FAl(OC_{10}F_{15})_3]^-$	-6192.42	1106.88	1.44975	-6199.29	-16275137.81
$[Al(OC_{10}F_{15})_4]^-$	-8042.83	1462.12	1.77949	-8051.82	-21138588.43
Cu^+	-1639.27	3.716358	0.16063	-1639.74	-4305132.17
H^+	0.00	3.716358	0.10886	0.00	6.20
$OCH(CF_3)_2^-$	-787.70	153.59	0.39341	-788.64	-2070407.42
$HCH(CF_3)_2$	-788.28	193.78	0.39524	-789.20	-2071849.36
$CuOCH(CF_3)_2$	-2427.26	166.45	0.43591	-2428.66	-6376269.60
$C_6F_5^-$	-726.36	148.43	0.37446	-727.17	-1909023.68
HC_6F_5	-726.96	185.76	0.37289	-727.75	-1910522.71
CuC_6F_5	-2365.93	160.45	0.42135	-2367.21	-6214938.53
$C_2F_5^-$	-574.29	76.97	0.33239	-574.98	-1509534.13

HC_2F_5	-574.91	118.48	0.33233	-575.59	-1511098.81
CuC_2F_5	-2213.87	89.73	0.37637	-2215.03	-5815472.64
$OC_5F_4N^-$	-718.48	153.92	0.37084	-719.28	-1888460.32
HOC_5F_4N	-719.00	189.44	0.37882	-719.80	-1889829.52
$CuOC_5F_4N$	-2357.99	163.02	0.42654	-2359.26	-6194247.34
$OC(CF_3)_3^-$	-1124.12	175.69	0.45845	-1125.44	-2954672.30
$HOC(CF_3)_3$	-1124.66	213.71	0.45808	-1125.98	-2956052.70
$CuOC(CF_3)_3$	-2763.65	187.15	0.50589	-2765.45	-7260487.94
$OTeF_5^-$	-841.45	59.53	0.36435	-841.95	-2210477.90
$HOTeF_5$	-841.96	92.51	0.37554	-842.45	-2211760.53
$CuOTeF_5$	-2480.96	68.2	0.41860	-2481.93	-6516231.09
$OC_{10}F_{15}^-$	-1950.14	351.89	0.56474	-1952.38	-5125619.55
$HOC_{10}F_{15}$	-1950.67	390.18	0.57567	-1952.91	-5126964.45
$CuOC_{10}F_{15}$	-3589.66	363.77	0.62008	-3592.37	-9431411.00

Detailed results for the calculation of the FIA

Me_3SiF

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c3v

Cartesian coordinates in Ångström:
Si          0.00000         0.00000         0.43489
C          -0.89942         1.55784        -0.12108
C          -0.89942        -1.55784        -0.12108
C           1.79883         0.00000        -0.12108
F          -0.00000         0.00000         2.08987
H          -0.93572         1.62071        -1.23198
H          -0.38849         2.47160         0.25570
H          -1.94622         1.57224         0.25570
H          -0.93572        -1.62071        -1.23198
H          -1.94622        -1.57224         0.25570
H          -0.38849        -2.47160         0.25570
H           1.87144         0.00000        -1.23198
H           2.33471        -0.89936         0.25570
H           2.33471         0.89936         0.25570

SCF energy GEOOPT =  -508.9440381828 H
ZPE =   289.2 kJ/mol
FREEH energy =   311.17 kJ/mol
FREEH entropy =   0.35193 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a2           150.98         0.00000       NO      NO
     8        e            168.61         0.00073       YES     YES
     9        e            168.61         0.00073       YES     YES
```

```
    10        e             187.21         0.02562       YES     YES
    11        e             187.21         0.02562       YES     YES
    12        a1            226.88         0.13168       YES     YES
    13        e             268.75        12.03584       YES     YES
    14        e             268.75        12.03584       YES     YES
    15        a1            589.22         0.03503       YES     YES
    16        a2            666.76         0.00000       NO      NO
    17        e             677.74         2.94282       YES     YES
    18        e             677.74         2.94282       YES     YES
    19        e             755.49        29.03448       YES     YES
    20        e             755.49        29.03448       YES     YES
    21        a1            771.60         4.00555       YES     YES
    22        e             853.29       137.16353       YES     YES
    23        e             853.29       137.16353       YES     YES
    24        a1            909.98       167.25528       YES     YES
    25        e            1245.74        47.70419       YES     YES
    26        e            1245.74        47.70419       YES     YES
    27        a1           1252.80        15.95531       YES     YES
    28        a2           1391.80         0.00000       NO      NO
    29        e            1399.37         0.05068       YES     YES
    30        e            1399.37         0.05068       YES     YES
    31        e            1405.49         4.82915       YES     YES
    32        e            1405.49         4.82915       YES     YES
    33        a1           1416.73        16.43413       YES     YES
    34        e            2942.01         3.43958       YES     YES
    35        e            2942.01         3.43958       YES     YES
    36        a1           2944.19         1.14242       YES     YES
    37        e            3033.32         0.60467       YES     YES
    38        e            3033.32         0.60467       YES     YES
    39        a1           3035.81        16.57344       YES     YES
    40        a2           3038.64         0.00000       NO      NO
    41        e            3039.33         8.82142       YES     YES
    42        e            3039.33         8.82142       YES     YES
$end
```

Me_3Si^+

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c3

Cartesian coordinates in Ångström:
Si        -0.00000       -0.00000       -0.00936
C         -1.77804       -0.49130       -0.00344
C          0.46354        1.78548       -0.00344
C          1.31450       -1.29418       -0.00344
H         -1.99314       -1.09661        0.91111
H         -1.98729       -1.16727       -0.86755
H         -2.47248        0.37431       -0.03700
H          0.04688        2.27442        0.91111
H         -0.01724        2.30468       -0.86755
H          1.56040        1.95407       -0.03700
H          1.94626       -1.17781        0.91111
H          2.00454       -1.13741       -0.86755
H          0.91207       -2.32839       -0.03700

SCF energy GEOOPT =  -408.8229091609 H
ZPE =   276.9 kJ/mol
FREEH energy =   297.88 kJ/mol
FREEH entropy =   0.35707 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                       -0.00         0.00000        -       -
     2                       -0.00         0.00000        -       -
     3                       -0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
```

```
     6                     0.00         0.00000        -       -
     7        e           45.70         0.01294       YES     YES
     8        e           45.70         0.01294       YES     YES
     9        a           74.04         2.66346       YES     YES
    10        e          209.09         2.15670       YES     YES
    11        e          209.09         2.15670       YES     YES
    12        a          214.70         1.27748       YES     YES
    13        a          594.46         0.01340       YES     YES
    14        e          621.77         0.01064       YES     YES
    15        e          621.77         0.01064       YES     YES
    16        a          694.79         0.00082       YES     YES
    17        e          743.84         7.60135       YES     YES
    18        e          743.84         7.60135       YES     YES
    19        a          817.60        83.69677       YES     YES
    20        e          883.78       133.61822       YES     YES
    21        e          883.78       133.61822       YES     YES
    22        e         1240.57        77.78588       YES     YES
    23        e         1240.57        77.78588       YES     YES
    24        a         1246.62         0.12967       YES     YES
    25        e         1360.16        11.89320       YES     YES
    26        e         1360.16        11.89320       YES     YES
    27        e         1362.24         0.13614       YES     YES
    28        e         1362.24         0.13614       YES     YES
    29        a         1366.22        21.97712       YES     YES
    30        a         1372.25        25.47705       YES     YES
    31        e         2925.07        45.87729       YES     YES
    32        e         2925.07        45.87729       YES     YES
    33        a         2930.25         0.18769       YES     YES
    34        a         3000.58        44.55103       YES     YES
    35        e         3000.94         0.02752       YES     YES
    36        e         3000.94         0.02752       YES     YES
    37        e         3066.31        14.37370       YES     YES
    38        e         3066.31        14.37370       YES     YES
    39        a         3066.92         0.00142       YES     YES
$end
```

$B(OCH(CF_3)_2)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
B         -0.00120       -0.00813       -0.02413
O         -0.14803       -1.25683        0.51956
O         -1.10474        0.70526       -0.41084
O          1.25052        0.52516       -0.18041
C          1.43577        1.80505       -0.73666
C          0.96923       -1.99109        0.96285
C         -2.40208        0.18394       -0.23920
C          2.15590        2.67671        0.31091
F          1.39467        2.72779        1.42540
F          3.35766        2.17798        0.64875
F          2.32325        3.93113       -0.14912
C          2.18769        1.64062       -2.07188
F          3.39086        1.06474       -1.90770
F          2.35878        2.83263       -2.67338
F          1.45230        0.85277       -2.88696
C          1.00823       -3.31314        0.17100
F          2.04963       -4.07244        0.56244
F         -0.12282       -4.02357        0.31655
F          1.15861       -3.02815       -1.14125
C          0.86074       -2.15272        2.49285
F         -0.20844       -2.88466        2.85115
F          0.73642       -0.92786        3.04977
F          1.96802       -2.73393        2.99082
C         -3.05500        0.05067       -1.62910
F         -2.28113       -0.74523       -2.39806
F         -3.18010        1.23709       -2.24806
```

F	-4.27404	-0.51226	-1.52626
C	-3.15660	1.10198	0.74236
F	-2.48217	1.13004	1.91308
F	-4.39684	0.63233	0.97635
F	-3.25238	2.36234	0.28549
H	0.46683	2.29909	-0.96475
H	1.92104	-1.45595	0.75762
H	-2.38055	-0.83137	0.21079

SCF energy GEOOPT = -2391.014017532 H
ZPE = 419.9 kJ/mol
FREEH energy = 497.71 kJ/mol
FREEH entropy = 0.88587 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.74	0.01989	YES	YES
8	a	11.24	0.04963	YES	YES
9	a	13.08	0.13736	YES	YES
10	a	15.02	0.03574	YES	YES
11	a	31.31	0.03296	YES	YES
12	a	32.71	0.00710	YES	YES
13	a	37.35	0.42764	YES	YES
14	a	37.84	0.38342	YES	YES
15	a	39.12	0.11923	YES	YES
16	a	45.76	0.00390	YES	YES
17	a	46.62	0.00111	YES	YES
18	a	61.96	0.00512	YES	YES
19	a	71.43	0.04769	YES	YES
20	a	73.00	0.02520	YES	YES
21	a	98.99	0.00065	YES	YES
22	a	145.06	4.48620	YES	YES
23	a	145.37	4.56460	YES	YES
24	a	166.58	0.00620	YES	YES
25	a	197.75	0.11784	YES	YES
26	a	199.25	0.03671	YES	YES
27	a	199.30	0.14315	YES	YES
28	a	247.87	1.25809	YES	YES
29	a	265.41	0.00043	YES	YES
30	a	266.54	0.00483	YES	YES
31	a	288.27	0.04062	YES	YES
32	a	288.47	0.02844	YES	YES
33	a	288.62	0.34107	YES	YES
34	a	318.43	1.63324	YES	YES
35	a	318.81	1.67598	YES	YES
36	a	323.52	0.00318	YES	YES
37	a	336.29	0.03434	YES	YES
38	a	357.01	0.00346	YES	YES
39	a	357.47	0.00460	YES	YES
40	a	375.05	0.47379	YES	YES
41	a	376.07	0.51584	YES	YES
42	a	417.78	0.00360	YES	YES
43	a	493.84	0.06816	YES	YES
44	a	494.08	0.08204	YES	YES
45	a	512.10	0.00786	YES	YES
46	a	521.91	0.33436	YES	YES
47	a	522.01	3.40193	YES	YES
48	a	522.87	2.38480	YES	YES
49	a	528.19	16.25014	YES	YES
50	a	528.60	16.41793	YES	YES
51	a	536.88	0.28950	YES	YES
52	a	536.96	1.42753	YES	YES
53	a	537.67	1.05658	YES	YES

54	a	554.70	0.00770	YES	YES
55	a	606.66	5.92112	YES	YES
56	a	636.71	24.48910	YES	YES
57	a	637.07	24.57316	YES	YES
58	a	674.25	0.58363	YES	YES
59	a	674.51	0.23866	YES	YES
60	a	676.54	126.57613	YES	YES
61	a	712.89	0.00295	YES	YES
62	a	728.31	20.04190	YES	YES
63	a	728.46	19.87048	YES	YES
64	a	852.26	0.03499	YES	YES
65	a	865.45	62.20989	YES	YES
66	a	865.81	62.84792	YES	YES
67	a	893.50	0.49069	YES	YES
68	a	897.77	7.18878	YES	YES
69	a	898.60	25.39200	YES	YES
70	a	899.76	68.00846	YES	YES
71	a	1096.00	8.58275	YES	YES
72	a	1098.29	7.39566	YES	YES
73	a	1106.18	457.85386	YES	YES
74	a	1108.50	143.90053	YES	YES
75	a	1109.60	141.23352	YES	YES
76	a	1164.96	0.29236	YES	YES
77	a	1166.12	0.55371	YES	YES
78	a	1171.12	12.97384	YES	YES
79	a	1174.89	0.26910	YES	YES
80	a	1202.93	127.78550	YES	YES
81	a	1204.50	134.24580	YES	YES
82	a	1209.59	1.68383	YES	YES
83	a	1217.08	665.66576	YES	YES
84	a	1218.29	685.00751	YES	YES
85	a	1239.29	1.04522	YES	YES
86	a	1248.49	317.17389	YES	YES
87	a	1249.51	1.30722	YES	YES
88	a	1250.27	25.43303	YES	YES
89	a	1278.11	656.25381	YES	YES
90	a	1278.38	654.88859	YES	YES
91	a	1284.07	1.69916	YES	YES
92	a	1354.44	5.58356	YES	YES
93	a	1362.26	37.98122	YES	YES
94	a	1363.17	27.24175	YES	YES
95	a	1363.40	74.94550	YES	YES
96	a	1369.76	26.24716	YES	YES
97	a	1370.09	157.96067	YES	YES
98	a	1433.74	701.07352	YES	YES
99	a	1435.59	706.71698	YES	YES
100	a	3008.33	8.50451	YES	YES
101	a	3009.57	10.05662	YES	YES
102	a	3013.06	10.04439	YES	YES

$end

$[FB(OCH(CF_3)_2)_3]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

B	0.17986	0.15103	0.03106
O	1.56615	0.09285	-0.44442
O	-0.42833	1.41765	-0.40854
O	-0.54396	-0.98749	-0.57084
C	2.24794	-1.07304	-0.16380
C	3.44073	-0.78964	0.77946
C	2.70416	-1.74190	-1.47950
F	3.04803	-0.06176	1.84123
F	4.44349	-0.11054	0.17133
F	3.97585	-1.94634	1.26104
F	3.44557	-2.86297	-1.23514

```
F          3.45881       -0.92400       -2.24488
F          1.64282       -2.11948       -2.21438
H          1.62147       -1.83318        0.35906
C         -0.54139        2.46071        0.47997
C         -2.03018        2.84228        0.63508
C          0.32486        3.65031        0.01484
C         -1.74892       -1.34657       -0.01113
C         -1.63881       -2.76566        0.59493
C         -2.85966       -1.25590       -1.07895
F          1.62484        3.29766       -0.00129
F         -0.00273        4.07950       -1.22285
F          0.20979        4.71955        0.85609
F         -2.21250        3.80054        1.58436
F         -2.57958        3.30019       -0.50876
F         -2.74762        1.76251        1.02836
F         -3.04016        0.02073       -1.46787
F         -4.05586       -1.70460       -0.59881
F         -2.57356       -1.98210       -2.18030
F         -2.73704       -3.09160        1.32834
F         -1.48256       -3.72644       -0.34426
F         -0.57395       -2.84036        1.42474
H         -0.18908        2.20001        1.50511
H         -2.06597       -0.68411        0.82750
F          0.11750        0.05216        1.45322

SCF energy GEOOPT =  -2490.922556363 H
ZPE =   420.9 kJ/mol
FREEH energy =   501.08 kJ/mol
FREEH entropy =   0.87361 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             13.31         0.13013       YES     YES
     8        a             18.48         0.09445       YES     YES
     9        a             21.42         0.22428       YES     YES
    10        a             26.84         0.23453       YES     YES
    11        a             34.65         0.03777       YES     YES
    12        a             35.85         0.05421       YES     YES
    13        a             37.71         0.05296       YES     YES
    14        a             43.37         0.11208       YES     YES
    15        a             50.26         0.00691       YES     YES
    16        a             61.77         0.16463       YES     YES
    17        a             67.65         0.10987       YES     YES
    18        a             72.02         0.06904       YES     YES
    19        a             90.93         0.47914       YES     YES
    20        a             97.95         0.16690       YES     YES
    21        a            109.12         0.04547       YES     YES
    22        a            141.99         0.18965       YES     YES
    23        a            149.94         1.58991       YES     YES
    24        a            153.63         0.80014       YES     YES
    25        a            181.83         0.46334       YES     YES
    26        a            193.55         0.16000       YES     YES
    27        a            197.25         0.37080       YES     YES
    28        a            210.86         1.69642       YES     YES
    29        a            228.51         2.99834       YES     YES
    30        a            237.42         4.78193       YES     YES
    31        a            278.49         0.71557       YES     YES
    32        a            284.75         0.19802       YES     YES
    33        a            285.59         0.16900       YES     YES
    34        a            286.35         0.16024       YES     YES
    35        a            288.42         0.26118       YES     YES
    36        a            301.55         0.13477       YES     YES
    37        a            320.60         1.44883       YES     YES
```

38	a	321.42	1.86788	YES	YES
39	a	322.74	0.14014	YES	YES
40	a	352.02	0.01780	YES	YES
41	a	377.47	0.39736	YES	YES
42	a	389.19	1.82879	YES	YES
43	a	441.21	6.94522	YES	YES
44	a	451.53	3.95458	YES	YES
45	a	497.81	3.03705	YES	YES
46	a	503.30	14.68855	YES	YES
47	a	505.35	8.71997	YES	YES
48	a	516.92	1.06264	YES	YES
49	a	519.70	3.28446	YES	YES
50	a	519.78	4.11298	YES	YES
51	a	520.80	3.76965	YES	YES
52	a	532.04	0.78983	YES	YES
53	a	533.00	0.43168	YES	YES
54	a	535.24	1.49666	YES	YES
55	a	535.54	1.46944	YES	YES
56	a	539.27	0.59572	YES	YES
57	a	595.02	1.38126	YES	YES
58	a	617.80	35.23713	YES	YES
59	a	630.63	33.36785	YES	YES
60	a	668.38	41.12379	YES	YES
61	a	670.11	25.32082	YES	YES
62	a	671.30	61.83719	YES	YES
63	a	703.58	3.93064	YES	YES
64	a	725.36	4.38235	YES	YES
65	a	727.61	2.75270	YES	YES
66	a	779.42	1.15964	YES	YES
67	a	851.70	12.18022	YES	YES
68	a	854.58	46.93205	YES	YES
69	a	859.19	58.88335	YES	YES
70	a	875.67	11.80951	YES	YES
71	a	876.37	36.96141	YES	YES
72	a	878.04	22.60377	YES	YES
73	a	1013.30	327.09548	YES	YES
74	a	1031.15	274.89518	YES	YES
75	a	1059.49	273.94780	YES	YES
76	a	1082.66	116.20396	YES	YES
77	a	1084.84	117.34491	YES	YES
78	a	1087.55	127.79840	YES	YES
79	a	1118.89	81.20033	YES	YES
80	a	1122.51	18.52085	YES	YES
81	a	1129.02	105.76320	YES	YES
82	a	1156.83	352.97316	YES	YES
83	a	1162.15	5.54054	YES	YES
84	a	1166.80	336.48793	YES	YES
85	a	1170.35	778.83573	YES	YES
86	a	1171.64	690.28827	YES	YES
87	a	1212.04	124.84770	YES	YES
88	a	1217.37	446.03719	YES	YES
89	a	1218.63	184.53025	YES	YES
90	a	1230.41	280.63586	YES	YES
91	a	1237.82	115.57589	YES	YES
92	a	1240.04	189.19221	YES	YES
93	a	1243.75	154.66618	YES	YES
94	a	1275.11	102.73052	YES	YES
95	a	1275.81	136.82160	YES	YES
96	a	1278.37	212.48365	YES	YES
97	a	1330.85	15.79472	YES	YES
98	a	1341.59	65.74645	YES	YES
99	a	1345.37	86.43407	YES	YES
100	a	1352.94	14.29842	YES	YES
101	a	1358.44	56.83946	YES	YES
102	a	1361.36	78.96146	YES	YES
103	a	2956.92	26.94941	YES	YES
104	a	2957.40	7.89158	YES	YES
105	a	2962.18	15.32962	YES	YES

$end

$B(C_6F_5)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C    -0.7494197   -3.8031110   -0.5638496
C    -0.8232391   -2.4036459   -0.6001268
C     0.1590028   -1.5689035   -0.0216491
C     1.2381688   -2.2254134    0.6101064
C     1.3384700   -3.6221520    0.6830067
C     0.3375385   -4.4118875    0.0891138
F    -1.8734367   -1.8680691   -1.2422257
F    -1.6912738   -4.5589373   -1.1340713
F     0.4198060   -5.7392342    0.1455499
F     2.3618041   -4.2088560    1.3084808
F     2.2061970   -1.5158034    1.2110960
C    -1.7775646    1.7702738   -0.6509510
C    -3.6164959    0.7189554    1.1710827
C    -1.3933215    0.6420872    0.1024650
C    -2.3516231    0.1378355    1.0059476
C    -3.9592959    1.8392121    0.3930742
C    -3.0394530    2.3687032   -0.5300434
F    -0.9311950    2.2987960   -1.5500509
F    -4.4919771    0.2277651    2.0515077
F    -3.3757664    3.4270296   -1.2716144
F    -5.1587974    2.4001913    0.5318374
F    -2.0593457   -0.9210356    1.7789870
C     2.3907843    0.5595063   -0.9884118
C     2.5056971    2.9757369    0.4130008
C     1.2860887    0.9094479   -0.1807568
C     1.3818161    2.1422608    0.5032517
C     3.5809720    2.5866703   -0.4058419
C     3.5255084    1.3734670   -1.1165181
F     2.3750200   -0.5785012   -1.6991702
F     2.5670695    4.1238506    1.0919573
F     4.5470115    1.0155699   -1.8984387
F     4.6548505    3.3666606   -0.5053876
F     0.3911823    2.5502330    1.3118676
B     0.0252171   -0.0087027   -0.0432255

SCF energy GEOOPT =  -2206.833883397 H
ZPE =   394.8 kJ/mol
FREEH energy =   472.69 kJ/mol
FREEH entropy =   0.81730 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              20.49         0.45799       YES     YES
     8        a              22.61         0.49103       YES     YES
     9        a              32.00         0.02360       YES     YES
    10        a              32.34         0.00730       YES     YES
    11        a              33.07         0.00098       YES     YES
    12        a              39.72         0.00303       YES     YES
    13        a             101.38         0.06245       YES     YES
    14        a             104.86         0.13161       YES     YES
    15        a             107.95         0.05756       YES     YES
    16        a             126.05         0.40123       YES     YES
    17        a             126.67         0.39881       YES     YES
    18        a             127.95         0.08298       YES     YES
    19        a             141.16         0.02950       YES     YES
    20        a             142.94         0.01926       YES     YES
```

21	a	147.82	0.00865	YES	YES
22	a	153.90	0.19590	YES	YES
23	a	155.53	0.15568	YES	YES
24	a	155.95	0.00557	YES	YES
25	a	222.45	3.71195	YES	YES
26	a	226.42	3.60508	YES	YES
27	a	229.25	3.68502	YES	YES
28	a	262.85	0.13637	YES	YES
29	a	263.11	0.17609	YES	YES
30	a	265.63	0.15395	YES	YES
31	a	270.00	0.20366	YES	YES
32	a	270.65	0.04690	YES	YES
33	a	272.68	0.07134	YES	YES
34	a	307.46	0.71462	YES	YES
35	a	308.14	0.29924	YES	YES
36	a	308.58	0.68820	YES	YES
37	a	340.45	2.68052	YES	YES
38	a	341.57	2.87219	YES	YES
39	a	345.63	0.07214	YES	YES
40	a	350.30	0.00331	YES	YES
41	a	376.49	5.98116	YES	YES
42	a	379.66	6.64442	YES	YES
43	a	392.69	1.07798	YES	YES
44	a	394.42	1.12428	YES	YES
45	a	395.21	0.58051	YES	YES
46	a	430.20	0.47530	YES	YES
47	a	431.40	0.25656	YES	YES
48	a	431.48	0.28082	YES	YES
49	a	460.21	4.76388	YES	YES
50	a	460.79	4.38519	YES	YES
51	a	486.94	0.00012	YES	YES
52	a	493.94	0.09435	YES	YES
53	a	506.02	0.01217	YES	YES
54	a	510.65	0.02169	YES	YES
55	a	534.10	1.89541	YES	YES
56	a	564.77	2.56602	YES	YES
57	a	565.20	2.89769	YES	YES
58	a	567.69	0.23577	YES	YES
59	a	617.75	26.21805	YES	YES
60	a	618.65	26.78201	YES	YES
61	a	632.57	1.80403	YES	YES
62	a	633.59	2.09773	YES	YES
63	a	635.58	0.06402	YES	YES
64	a	664.01	23.42541	YES	YES
65	a	667.14	24.84175	YES	YES
66	a	675.98	6.75737	YES	YES
67	a	770.59	21.98469	YES	YES
68	a	771.09	21.66480	YES	YES
69	a	774.81	6.35942	YES	YES
70	a	857.28	0.05522	YES	YES
71	a	985.45	166.27271	YES	YES
72	a	986.47	65.73133	YES	YES
73	a	987.76	74.24824	YES	YES
74	a	1026.11	127.64715	YES	YES
75	a	1026.49	119.17287	YES	YES
76	a	1119.95	0.20792	YES	YES
77	a	1156.10	7.59198	YES	YES
78	a	1159.29	16.01727	YES	YES
79	a	1160.09	15.74119	YES	YES
80	a	1186.80	181.40243	YES	YES
81	a	1190.04	194.43842	YES	YES
82	a	1306.70	0.67193	YES	YES
83	a	1320.59	152.87727	YES	YES
84	a	1323.85	177.00502	YES	YES
85	a	1349.99	0.89668	YES	YES
86	a	1353.63	4.81481	YES	YES
87	a	1356.76	6.56161	YES	YES
88	a	1384.79	335.27637	YES	YES
89	a	1388.42	278.96068	YES	YES
90	a	1403.51	10.77157	YES	YES

91	a	1476.15	458.01026	YES	YES
92	a	1485.66	657.52127	YES	YES
93	a	1487.54	592.38301	YES	YES
94	a	1522.14	248.22444	YES	YES
95	a	1523.17	198.28540	YES	YES
96	a	1525.59	54.79670	YES	YES
97	a	1611.29	17.59635	YES	YES
98	a	1613.47	8.38797	YES	YES
99	a	1617.05	8.45321	YES	YES
100	a	1633.04	188.72941	YES	YES
101	a	1634.17	115.04625	YES	YES
102	a	1637.97	92.01546	YES	YES

$end

$[FB(C_6F_5)_3]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

C	-0.6324775	-3.6701425	-0.7346613
C	-0.7454505	-2.2933128	-0.4618159
C	0.1764473	-1.5853953	0.3198383
C	1.2649751	-2.3397873	0.7899923
C	1.4259284	-3.7118214	0.5406740
C	0.4623198	-4.3834716	-0.2281699
F	-1.8139118	-1.6795451	-1.0203839
F	-1.5580113	-4.3086968	-1.4782899
F	0.5920852	-5.6999337	-0.4796236
F	2.4930756	-4.3886400	1.0098680
F	2.2472589	-1.7443199	1.4962813
C	-1.6542380	1.6019578	-0.5945823
C	-3.7964434	0.8430243	1.0042582
C	-1.4013388	0.6587668	0.4101982
C	-2.5176174	0.2891427	1.1789776
C	-3.9946276	1.8042283	0.0013010
C	-2.9159271	2.1870113	-0.8073008
F	-0.6787678	2.0042354	-1.4419140
F	-4.8373204	0.4584567	1.7693030
F	-3.1023750	3.1036727	-1.7773451
F	-5.2112361	2.3501769	-0.1839592
F	-2.4061274	-0.6629396	2.1262591
C	2.1797318	0.5279111	-0.8834158
C	2.5770061	3.0258611	0.2677190
C	1.2994348	0.9105161	0.1362690
C	1.5237049	2.1897225	0.6708713
C	3.4505127	2.5869047	-0.7389920
C	3.2503923	1.3282017	-1.3225750
F	2.0372764	-0.6546493	-1.5256265
F	2.7503777	4.2447591	0.8155990
F	4.0784678	0.9066319	-2.2992712
F	4.4700480	3.3693038	-1.1412284
F	0.6907711	2.6918683	1.6050905
B	0.0730324	0.0021221	0.7763195
F	0.2230238	0.0381797	2.2003357

SCF energy GEOOPT = -2306.760365259 H
ZPE = 397.2 kJ/mol
FREEH energy = 478.69 kJ/mol
FREEH entropy = 0.84713 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.10	0.00184	YES	YES
8	a	17.88	0.00532	YES	YES
9	a	25.10	0.02048	YES	YES
10	a	29.76	0.02972	YES	YES
11	a	30.59	0.03285	YES	YES
12	a	41.52	0.04715	YES	YES
13	a	101.36	0.28537	YES	YES
14	a	102.88	0.10195	YES	YES
15	a	104.82	0.24818	YES	YES
16	a	121.81	0.02562	YES	YES
17	a	123.42	0.02115	YES	YES
18	a	128.70	0.00888	YES	YES
19	a	137.14	0.02703	YES	YES
20	a	143.33	0.23329	YES	YES
21	a	146.34	0.22532	YES	YES
22	a	156.24	0.01858	YES	YES
23	a	159.58	0.14510	YES	YES
24	a	161.65	0.11133	YES	YES
25	a	208.55	2.91182	YES	YES
26	a	212.85	2.96454	YES	YES
27	a	221.39	1.63047	YES	YES
28	a	244.67	0.56582	YES	YES
29	a	247.16	0.67127	YES	YES
30	a	260.67	0.03677	YES	YES
31	a	263.14	0.08256	YES	YES
32	a	265.16	0.07216	YES	YES
33	a	270.22	0.07109	YES	YES
34	a	273.14	0.06670	YES	YES
35	a	273.86	0.05706	YES	YES
36	a	305.17	0.43253	YES	YES
37	a	307.92	0.66173	YES	YES
38	a	309.12	0.58177	YES	YES
39	a	309.64	0.25799	YES	YES
40	a	344.15	3.06103	YES	YES
41	a	344.50	3.11264	YES	YES
42	a	347.04	0.02836	YES	YES
43	a	384.42	0.39849	YES	YES
44	a	385.70	0.47300	YES	YES
45	a	386.44	1.26171	YES	YES
46	a	390.23	1.38683	YES	YES
47	a	391.15	0.41113	YES	YES
48	a	432.61	0.47780	YES	YES
49	a	434.15	0.14071	YES	YES
50	a	434.49	0.14123	YES	YES
51	a	434.70	0.14516	YES	YES
52	a	466.66	1.82803	YES	YES
53	a	467.09	1.87896	YES	YES
54	a	484.19	0.01367	YES	YES
55	a	492.53	0.08598	YES	YES
56	a	495.76	0.00397	YES	YES
57	a	504.44	0.01362	YES	YES
58	a	562.86	3.20482	YES	YES
59	a	563.56	2.99615	YES	YES
60	a	564.97	0.52741	YES	YES
61	a	604.29	31.48745	YES	YES
62	a	607.28	34.07671	YES	YES
63	a	627.39	0.15006	YES	YES
64	a	628.56	0.26857	YES	YES
65	a	630.97	0.17821	YES	YES
66	a	640.56	0.23337	YES	YES
67	a	692.08	68.51928	YES	YES
68	a	696.26	73.18927	YES	YES
69	a	744.79	2.83023	YES	YES
70	a	759.68	36.04332	YES	YES
71	a	760.52	35.30719	YES	YES
72	a	814.36	5.25564	YES	YES
73	a	932.87	8.36894	YES	YES
74	a	936.86	7.52362	YES	YES

75	a	966.43	291.83589	YES	YES
76	a	980.90	151.18098	YES	YES
77	a	981.75	141.47759	YES	YES
78	a	999.75	0.48949	YES	YES
79	a	1086.77	29.73572	YES	YES
80	a	1095.78	324.15094	YES	YES
81	a	1096.72	317.68746	YES	YES
82	a	1130.00	0.86305	YES	YES
83	a	1132.25	1.04682	YES	YES
84	a	1132.80	0.96335	YES	YES
85	a	1265.11	63.92020	YES	YES
86	a	1265.65	35.23415	YES	YES
87	a	1269.51	39.79747	YES	YES
88	a	1352.99	6.20409	YES	YES
89	a	1356.57	5.73127	YES	YES
90	a	1357.24	7.75681	YES	YES
91	a	1379.84	22.36353	YES	YES
92	a	1380.40	23.18619	YES	YES
93	a	1387.94	1.38091	YES	YES
94	a	1464.68	479.08984	YES	YES
95	a	1470.10	492.94709	YES	YES
96	a	1470.32	425.66760	YES	YES
97	a	1507.87	205.45739	YES	YES
98	a	1509.75	198.30698	YES	YES
99	a	1512.64	23.49859	YES	YES
100	a	1619.04	2.83068	YES	YES
101	a	1621.78	2.39206	YES	YES
102	a	1622.64	0.76906	YES	YES
103	a	1625.56	53.68739	YES	YES
104	a	1627.30	54.63993	YES	YES
105	a	1629.23	15.09761	YES	YES

$end

$Ga(C_2F_5)_3$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

Ga	-0.0101844	-0.0392630	0.1827376
F	-0.0748567	1.4329214	-2.2620484
F	1.1204726	-0.4199799	-2.4309707
F	1.8031251	1.8941190	0.0744971
F	2.2998988	2.4416622	-1.9932623
F	3.1162287	0.6123636	-1.1293092
C	0.7710412	0.5973913	-1.5890895
C	2.0404570	1.4036221	-1.1995190
F	2.2706845	-1.4780226	1.2791610
F	0.4004284	-1.7070323	2.4384950
F	1.4616680	-3.1222178	-0.5537520
F	0.2200556	-3.8883526	1.0683136
F	-0.6199342	-2.4459912	-0.3610288
C	0.9131207	-1.5579558	1.1788078
C	0.5262702	-2.8137651	0.3461392
F	-2.4436374	-0.3417154	1.5259041
F	-1.2619225	1.4079041	2.2175058
F	-2.8842078	0.9560554	-0.8845446
F	-3.6433917	2.0278864	0.8665630
F	-1.8162548	2.7123080	-0.1204058
C	-1.6589735	0.7028965	1.1089552
C	-2.5300879	1.6251658	0.2368509

SCF energy GEOOPT = -3649.965532910 H
ZPE = 199.2 kJ/mol
FREEH energy = 260.03 kJ/mol
FREEH entropy = 0.72732 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.70	0.00316	YES	YES
8	a	17.10	0.18268	YES	YES
9	a	27.77	0.08139	YES	YES
10	a	34.02	0.41656	YES	YES
11	a	44.72	0.50645	YES	YES
12	a	47.65	0.45221	YES	YES
13	a	53.57	0.42400	YES	YES
14	a	54.71	1.03293	YES	YES
15	a	62.86	0.14243	YES	YES
16	a	80.65	1.63601	YES	YES
17	a	99.34	6.87584	YES	YES
18	a	111.81	9.11909	YES	YES
19	a	170.52	0.43228	YES	YES
20	a	183.65	0.44239	YES	YES
21	a	205.34	1.41173	YES	YES
22	a	209.07	0.03962	YES	YES
23	a	216.51	6.07546	YES	YES
24	a	227.93	0.77553	YES	YES
25	a	230.40	2.08841	YES	YES
26	a	258.91	7.03139	YES	YES
27	a	275.88	7.51634	YES	YES
28	a	286.53	7.47059	YES	YES
29	a	311.02	23.62869	YES	YES
30	a	318.73	29.99805	YES	YES
31	a	356.68	0.78334	YES	YES
32	a	362.70	0.99194	YES	YES
33	a	364.54	2.56421	YES	YES
34	a	408.06	0.55766	YES	YES
35	a	413.44	3.28194	YES	YES
36	a	417.59	0.07352	YES	YES
37	a	518.00	1.34921	YES	YES
38	a	520.93	0.48731	YES	YES
39	a	522.15	1.48961	YES	YES
40	a	558.54	4.44352	YES	YES
41	a	561.98	3.41482	YES	YES
42	a	570.76	1.73552	YES	YES
43	a	591.81	4.13236	YES	YES
44	a	595.56	1.97627	YES	YES
45	a	597.68	10.85494	YES	YES
46	a	706.67	17.46512	YES	YES
47	a	711.55	20.15514	YES	YES
48	a	722.41	16.86659	YES	YES
49	a	894.73	5.14125	YES	YES
50	a	904.44	52.64952	YES	YES
51	a	940.29	72.70629	YES	YES
52	a	1036.96	197.03828	YES	YES
53	a	1061.79	165.72787	YES	YES
54	a	1075.34	157.00394	YES	YES
55	a	1092.74	50.23999	YES	YES
56	a	1102.08	104.40905	YES	YES
57	a	1111.98	232.24469	YES	YES
58	a	1139.88	39.74263	YES	YES
59	a	1148.41	98.00044	YES	YES
60	a	1182.86	235.28473	YES	YES
61	a	1203.67	151.68464	YES	YES
62	a	1241.49	197.93877	YES	YES
63	a	1251.92	244.67034	YES	YES
64	a	1280.98	462.99038	YES	YES
65	a	1284.80	324.49425	YES	YES
66	a	1305.11	19.22728	YES	YES

$end

$[FGa(C_2F_5)_3]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Ga   -0.5794431   -0.4140866   -0.2155154
F    -0.1356668    1.5305282   -2.2582354
F     1.0394472   -0.3244987   -2.5742325
F     1.5517795    2.1206037   -0.0772670
F     2.4934704    1.9836729   -2.0448999
F     2.7519094    0.3706670   -0.5976651
C     0.6005876    0.5559018   -1.5978490
C     1.8623672    1.2649259   -1.0785235
F     1.4656436   -0.9829854    1.7001203
F    -0.3738981   -2.1915409    2.0110410
F     1.9762881   -2.4860697   -0.6116122
F     1.9083693   -3.5928703    1.2707488
F     0.2473049   -3.7370517   -0.1375056
C     0.4634878   -1.6740681    1.0326156
C     1.1543251   -2.8856205    0.3854369
F    -2.7303318    0.1306024    1.5737174
F    -0.8657794    1.2032271    2.1296823
F    -2.9899482    1.8392689   -0.6218646
F    -2.9889187    2.7974236    1.3412615
F    -1.2271444    2.9402877    0.0622050
C    -1.6449069    0.8136655    1.0480496
C    -2.2180986    2.1107636    0.4539986
F    -1.7608442   -1.3727464   -1.1937069

SCF energy GEOOPT =  -3749.904064578 H
ZPE =   203.2 kJ/mol
FREEH energy =   267.45 kJ/mol
FREEH entropy =   0.73042 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             24.94         0.01697       YES     YES
     8        a             30.27         0.14377       YES     YES
     9        a             42.55         0.03894       YES     YES
    10        a             44.06         0.04496       YES     YES
    11        a             47.88         0.06121       YES     YES
    12        a             53.73         0.09179       YES     YES
    13        a             62.14         0.17598       YES     YES
    14        a             72.15         0.02832       YES     YES
    15        a             77.12         0.09752       YES     YES
    16        a             96.06         1.22481       YES     YES
    17        a            103.60         0.36336       YES     YES
    18        a            111.45         2.77395       YES     YES
    19        a            136.84         9.04073       YES     YES
    20        a            140.78         3.20992       YES     YES
    21        a            190.25         0.87352       YES     YES
    22        a            192.75         0.48322       YES     YES
    23        a            206.49         0.71862       YES     YES
    24        a            212.22         0.68764       YES     YES
    25        a            212.60         0.38469       YES     YES
    26        a            217.31         0.17676       YES     YES
    27        a            235.09         5.17080       YES     YES
    28        a            252.47        15.12391       YES     YES
    29        a            267.05         1.37022       YES     YES
    30        a            274.54         1.59438       YES     YES
    31        a            289.09        37.22345       YES     YES
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    32        a             302.98        45.01348       YES     YES
    33        a             353.99         0.82170       YES     YES
    34        a             356.07         0.37124       YES     YES
    35        a             357.32         2.69686       YES     YES
    36        a             414.74         0.74020       YES     YES
    37        a             419.39         0.16778       YES     YES
    38        a             420.30         0.51058       YES     YES
    39        a             515.73         1.23527       YES     YES
    40        a             517.26         1.11330       YES     YES
    41        a             518.57         0.31882       YES     YES
    42        a             567.48         3.00057       YES     YES
    43        a             568.86         1.07568       YES     YES
    44        a             569.47         3.41030       YES     YES
    45        a             581.37         2.03608       YES     YES
    46        a             585.53         3.85885       YES     YES
    47        a             587.94         0.01656       YES     YES
    48        a             618.56        48.65124       YES     YES
    49        a             715.11        19.79332       YES     YES
    50        a             716.07        10.00110       YES     YES
    51        a             716.85         8.85352       YES     YES
    52        a             912.22       102.81189       YES     YES
    53        a             916.66        56.05685       YES     YES
    54        a             925.20         7.83014       YES     YES
    55        a            1014.68        40.17865       YES     YES
    56        a            1022.66        96.11498       YES     YES
    57        a            1030.67       208.75546       YES     YES
    58        a            1085.31        13.65827       YES     YES
    59        a            1090.19        40.83687       YES     YES
    60        a            1095.77       227.66195       YES     YES
    61        a            1153.95       218.64752       YES     YES
    62        a            1158.34       622.97739       YES     YES
    63        a            1158.95        46.77729       YES     YES
    64        a            1172.75        82.04545       YES     YES
    65        a            1189.05       449.92094       YES     YES
    66        a            1197.81        94.92013       YES     YES
    67        a            1268.82       406.44152       YES     YES
    68        a            1280.31       146.91297       YES     YES
    69        a            1295.22        16.31665       YES     YES
$end
```

$B(OC_5F_4N)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c3

Cartesian coordinates in Ångström:
B         -0.00000        0.00000       -0.04115
O         -1.37143        0.00042       -0.02115
C         -2.08540       -1.16080       -0.01413
C         -2.69259       -1.60123        1.17562
C         -3.44914       -2.78494        1.12050
N         -3.60138       -3.48776        0.01387
C         -3.02685       -3.08752       -1.10495
C         -2.24806       -1.92034       -1.18697
F         -2.52638       -0.90862        2.30470
F         -1.65700       -1.52919       -2.31977
F         -3.19842       -3.83135       -2.19794
F         -4.03759       -3.22923        2.23111
O          0.68535       -1.18790       -0.02115
O          0.68608        1.18748       -0.02115
C          0.03742        2.38640       -0.01413
C          2.04798       -1.22561       -0.01413
C         -0.04041        3.13246        1.17562
C         -0.68726        4.37952        1.12050
N         -1.21980        4.86276        0.01387
C         -1.16044        4.16509       -1.10495
C         -0.53904        2.90705       -1.18697
C          2.78710       -0.98671       -1.18697
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C          4.18730       -1.07757       -1.10495
N          4.82118       -1.37501        0.01387
C          4.13640       -1.59457        1.12050
C          2.73300       -1.53123        1.17562
F         -1.71884        4.68559       -2.19794
F         -0.49581        2.19960       -2.31977
F         -0.77780        5.11127        2.23111
F          0.47630        2.64222        2.30470
F          2.05008       -1.73360        2.30470
F          4.81539       -1.88204        2.23111
F          4.91726       -0.85424       -2.19794
F          2.15282       -0.67041       -2.31977

SCF energy GEOOPT =  -2183.114209757 H
ZPE =   407.1 kJ/mol
FREEH energy =   482.91 kJ/mol
FREEH entropy =   0.84514 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a              8.43         0.00029       YES     YES
     8        e              9.91         0.00396       YES     YES
     9        e              9.91         0.00396       YES     YES
    10        a             16.03         0.18963       YES     YES
    11        e             25.28         0.18480       YES     YES
    12        e             25.28         0.18480       YES     YES
    13        e             41.07         0.01835       YES     YES
    14        e             41.07         0.01835       YES     YES
    15        a             62.42         0.01035       YES     YES
    16        e            108.98         0.26556       YES     YES
    17        e            108.98         0.26556       YES     YES
    18        a            112.15         0.00408       YES     YES
    19        e            114.36         0.10361       YES     YES
    20        e            114.36         0.10361       YES     YES
    21        a            120.81         0.00027       YES     YES
    22        e            206.39         3.47541       YES     YES
    23        e            206.39         3.47541       YES     YES
    24        a            211.85         0.25671       YES     YES
    25        e            258.40         2.64854       YES     YES
    26        e            258.40         2.64854       YES     YES
    27        a            263.72         0.03759       YES     YES
    28        a            270.79         0.07930       YES     YES
    29        e            282.18         0.41091       YES     YES
    30        e            282.18         0.41091       YES     YES
    31        e            298.41         0.80745       YES     YES
    32        e            298.41         0.80745       YES     YES
    33        a            306.00         0.39004       YES     YES
    34        a            328.27         0.14863       YES     YES
    35        e            330.44         0.95946       YES     YES
    36        e            330.44         0.95946       YES     YES
    37        e            347.00         0.03459       YES     YES
    38        e            347.00         0.03459       YES     YES
    39        a            358.10         0.20355       YES     YES
    40        e            406.09         1.51467       YES     YES
    41        e            406.09         1.51467       YES     YES
    42        a            432.13         0.00482       YES     YES
    43        e            432.42         0.11185       YES     YES
    44        e            432.42         0.11185       YES     YES
    45        a            445.51         0.03654       YES     YES
    46        e            447.18         0.05352       YES     YES
    47        e            447.18         0.05352       YES     YES
    48        a            458.21         0.23414       YES     YES
    49        e            501.10         9.00206       YES     YES
```

50	e	501.10	9.00206	YES	YES
51	a	541.12	0.61767	YES	YES
52	a	595.15	12.99734	YES	YES
53	e	598.88	13.63216	YES	YES
54	e	598.88	13.63216	YES	YES
55	a	625.13	0.02527	YES	YES
56	e	647.88	0.07268	YES	YES
57	e	647.88	0.07268	YES	YES
58	e	648.60	0.02570	YES	YES
59	e	648.60	0.02570	YES	YES
60	a	648.71	0.19391	YES	YES
61	a	664.78	0.43158	YES	YES
62	e	674.64	6.33343	YES	YES
63	e	674.64	6.33343	YES	YES
64	a	677.26	0.02902	YES	YES
65	e	696.70	7.53229	YES	YES
66	e	696.70	7.53229	YES	YES
67	a	729.34	0.01693	YES	YES
68	e	732.02	0.24362	YES	YES
69	e	732.02	0.24362	YES	YES
70	a	843.24	0.54232	YES	YES
71	e	981.02	13.65347	YES	YES
72	e	981.02	13.65347	YES	YES
73	a	984.01	408.09249	YES	YES
74	e	1074.25	374.78352	YES	YES
75	e	1074.25	374.78352	YES	YES
76	a	1144.16	0.31483	YES	YES
77	e	1177.91	0.56698	YES	YES
78	e	1177.91	0.56698	YES	YES
79	a	1181.75	2.62511	YES	YES
80	e	1279.85	13.49934	YES	YES
81	e	1279.85	13.49934	YES	YES
82	a	1304.69	0.33496	YES	YES
83	e	1375.04	33.39361	YES	YES
84	e	1375.04	33.39361	YES	YES
85	a	1375.48	65.95236	YES	YES
86	e	1389.96	1109.83764	YES	YES
87	e	1389.96	1109.83764	YES	YES
88	a	1441.02	0.00006	YES	YES
89	e	1442.15	9.13908	YES	YES
90	e	1442.15	9.13908	YES	YES
91	e	1499.01	55.37544	YES	YES
92	e	1499.01	55.37544	YES	YES
93	a	1505.28	1590.78802	YES	YES
94	e	1518.80	482.41397	YES	YES
95	e	1518.80	482.41397	YES	YES
96	a	1526.90	1.95799	YES	YES
97	e	1622.55	122.70718	YES	YES
98	e	1622.55	122.70718	YES	YES
99	a	1627.09	0.00151	YES	YES
100	e	1637.07	0.64167	YES	YES
101	e	1637.07	0.64167	YES	YES
102	a	1637.44	19.78621	YES	YES

$end

$[FB(OC_5F_4N)_3]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c3

Cartesian coordinates in Ångström:

B	-0.00000	-0.00000	1.90174
O	-1.38973	0.08088	1.36042
C	-1.92949	-0.83357	0.57310
C	-2.13554	-2.18160	0.96550
C	-2.73383	-3.06578	0.06025
N	-3.13726	-2.72186	-1.15105
C	-2.95571	-1.47108	-1.53694

```
C         -2.36171       -0.49044       -0.73335
F         -1.77329       -2.59054        2.18778
F         -2.18249        0.76214       -1.18624
F         -3.36648       -1.14162       -2.77529
F         -2.92955       -4.34456        0.43462
O          0.62482       -1.24398        1.36042
O          0.76491        1.16310        1.36042
C          0.24285        2.08777        0.57310
C          1.68663       -1.25420        0.57310
C         -0.82155        2.94023        0.96550
C         -1.28812        3.90046        0.06025
N         -0.78857        4.07788       -1.15105
C          0.20386        3.29526       -1.53694
C          0.75612        2.29052       -0.73335
C          1.60559       -1.80008       -0.73335
C          2.75185       -1.82418       -1.53694
N          3.92583       -1.35602       -1.15105
C          4.02196       -0.83468        0.06025
C          2.95709       -0.75863        0.96550
F          0.69457        3.48626       -2.77529
F          1.75128        1.50902       -1.18624
F         -2.29773        4.70934        0.43462
F         -1.35683        2.83098        2.18778
F          3.13012       -0.24044        2.18778
F          5.22727       -0.36478        0.43462
F          2.67191       -2.34464       -2.77529
F          0.43121       -2.27116       -1.18624
F          0.00000       -0.00000        3.27547

SCF energy GEOOPT =  -2283.057708689 H
ZPE =   409.4 kJ/mol
FREEH energy =   488.00 kJ/mol
FREEH entropy =   0.83021 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000         -       -
     2                      -0.00         0.00000         -       -
     3                      -0.00         0.00000         -       -
     4                      -0.00         0.00000         -       -
     5                      -0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
     7        e             17.48         0.02482       YES     YES
     8        e             17.48         0.02482       YES     YES
     9        a             19.76         0.00172       YES     YES
    10        a             27.61         0.09368       YES     YES
    11        e             32.78         0.03317       YES     YES
    12        e             32.78         0.03317       YES     YES
    13        e             54.59         0.64190       YES     YES
    14        e             54.59         0.64190       YES     YES
    15        a             71.92         0.15278       YES     YES
    16        e            111.28         0.22634       YES     YES
    17        e            111.28         0.22634       YES     YES
    18        a            113.79         0.04923       YES     YES
    19        e            120.45         0.13618       YES     YES
    20        e            120.45         0.13618       YES     YES
    21        a            124.46         0.01184       YES     YES
    22        e            197.83         0.96497       YES     YES
    23        e            197.83         0.96497       YES     YES
    24        a            208.22         0.84548       YES     YES
    25        e            217.77         0.91921       YES     YES
    26        e            217.77         0.91921       YES     YES
    27        e            241.81         0.06461       YES     YES
    28        e            241.81         0.06461       YES     YES
    29        a            262.93         0.00065       YES     YES
    30        a            274.14         0.00725       YES     YES
    31        e            278.60         0.65898       YES     YES
    32        e            278.60         0.65898       YES     YES
    33        e            297.32         0.06854       YES     YES
```

34	e	297.32	0.06854	YES	YES
35	a	306.06	0.38253	YES	YES
36	a	333.86	1.27833	YES	YES
37	e	345.16	0.23565	YES	YES
38	e	345.16	0.23565	YES	YES
39	a	355.51	0.22692	YES	YES
40	e	360.24	3.80386	YES	YES
41	e	360.24	3.80386	YES	YES
42	e	429.20	0.51191	YES	YES
43	e	429.20	0.51191	YES	YES
44	a	432.12	0.11245	YES	YES
45	e	432.18	1.01462	YES	YES
46	e	432.18	1.01462	YES	YES
47	a	439.43	2.08918	YES	YES
48	a	454.56	0.57780	YES	YES
49	e	458.70	1.44583	YES	YES
50	e	458.70	1.44583	YES	YES
51	a	483.24	7.55187	YES	YES
52	e	500.89	0.51072	YES	YES
53	e	500.89	0.51072	YES	YES
54	a	539.31	0.14941	YES	YES
55	e	610.05	33.12815	YES	YES
56	e	610.05	33.12815	YES	YES
57	a	629.46	0.15371	YES	YES
58	e	633.71	0.19749	YES	YES
59	e	633.71	0.19749	YES	YES
60	a	634.18	0.12054	YES	YES
61	e	635.92	1.14871	YES	YES
62	e	635.92	1.14871	YES	YES
63	a	657.65	0.90606	YES	YES
64	e	664.30	1.99118	YES	YES
65	e	664.30	1.99118	YES	YES
66	a	679.19	2.31640	YES	YES
67	e	687.05	6.33363	YES	YES
68	e	687.05	6.33363	YES	YES
69	a	721.55	0.38951	YES	YES
70	e	730.18	0.61411	YES	YES
71	e	730.18	0.61411	YES	YES
72	a	757.13	5.34512	YES	YES
73	e	913.45	348.93943	YES	YES
74	e	913.45	348.93943	YES	YES
75	a	969.13	209.29546	YES	YES
76	e	972.59	277.61161	YES	YES
77	e	972.59	277.61161	YES	YES
78	e	1114.68	500.36471	YES	YES
79	e	1114.68	500.36471	YES	YES
80	a	1130.57	68.81042	YES	YES
81	a	1147.69	71.56453	YES	YES
82	e	1148.75	12.22248	YES	YES
83	e	1148.75	12.22248	YES	YES
84	a	1179.13	533.01547	YES	YES
85	e	1302.12	0.86952	YES	YES
86	e	1302.12	0.86952	YES	YES
87	a	1310.47	33.64466	YES	YES
88	e	1376.14	5.25655	YES	YES
89	e	1376.14	5.25655	YES	YES
90	a	1376.60	20.04735	YES	YES
91	e	1418.72	37.82167	YES	YES
92	e	1418.72	37.82167	YES	YES
93	a	1421.02	13.50730	YES	YES
94	e	1484.14	372.75759	YES	YES
95	e	1484.14	372.75759	YES	YES
96	a	1485.03	733.27256	YES	YES
97	e	1533.12	426.19329	YES	YES
98	e	1533.12	426.19329	YES	YES
99	a	1551.27	198.11302	YES	YES
100	e	1607.74	3.52343	YES	YES
101	e	1607.74	3.52343	YES	YES
102	a	1607.86	2.52630	YES	YES
103	e	1624.28	171.24094	YES	YES

```
   104        e            1624.28       171.24094       YES     YES
   105        a            1635.03       130.82539       YES     YES
$end
```

$Al(OC(CF_3)_3)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Al    0.1004937    0.0055692    0.1595586
O     1.7538020    0.0799153    0.7504639
O    -0.8338041    1.4386102    0.2475055
O    -0.4916177   -1.5794630   -0.3036040
C    -0.9604161   -2.5201214    0.5769706
C     2.8422499    0.2559631   -0.0615260
C    -1.7716754    2.2274387   -0.3554455
C    -0.3306876   -3.9113393    0.2097376
F     0.9888730   -3.7760330    0.0093230
F    -0.8783174   -4.3974918   -0.9140124
F    -0.5256844   -4.8056243    1.2030949
C    -0.5412980   -2.1348618    2.0492006
F    -1.3904940   -2.4911095    2.9990432
F    -0.4886923   -0.7080253    2.0701549
F     0.6830027   -2.5355254    2.3725340
C    -2.5287116   -2.5695631    0.4747031
F    -2.9052504   -2.6102978   -0.8059506
F    -3.0429050   -1.4474623    1.0280596
F    -3.0458006   -3.6343762    1.1158393
C     3.2724574    1.7678419   -0.0266123
F     2.3601315    2.5032241   -0.7053288
F     4.4777917    1.9630932   -0.5929124
F     3.3060467    2.2097058    1.2326258
C     4.0070177   -0.6679815    0.4442329
F     4.9747146   -0.7768493   -0.4932028
F     3.5349960   -1.8933465    0.7132079
F     4.5520230   -0.1697714    1.5640499
C     2.4691267   -0.1488052   -1.5373676
F     1.0808431    0.1887775   -1.6828258
F     2.5312885   -1.4556277   -1.7577928
F     3.1059675    0.4986569   -2.4967577
C    -2.8398259    2.6313106    0.7256433
F    -3.9457294    3.1488812    0.1557669
F    -2.3339296    3.5448791    1.5741616
F    -3.1923217    1.5540544    1.4453940
C    -1.0525122    3.5099928   -0.9154096
F    -1.9280791    4.4762038   -1.2459996
F    -0.3395526    3.1863549   -2.0183721
F    -0.1986214    3.9968455   -0.0067232
C    -2.4727402    1.4547642   -1.5325789
F    -1.5422021    0.7289825   -2.2004199
F    -3.0725814    2.2755038   -2.4062102
F    -3.3873756    0.5871071   -1.0622191

SCF energy GEOOPT =  -3619.006939586 H
ZPE =   433.6 kJ/mol
FREEH energy =   541.91 kJ/mol
FREEH entropy =   1.05638 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000         -       -
     2                       0.00         0.00000         -       -
     3                       0.00         0.00000         -       -
     4                       0.00         0.00000         -       -
     5                       0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
```

7	a	16.38	0.03420	YES	YES
8	a	19.52	0.01833	YES	YES
9	a	23.89	0.01431	YES	YES
10	a	26.26	0.07586	YES	YES
11	a	29.17	0.02025	YES	YES
12	a	33.99	0.03181	YES	YES
13	a	42.61	0.10081	YES	YES
14	a	58.80	0.99275	YES	YES
15	a	63.38	0.05203	YES	YES
16	a	65.16	0.20241	YES	YES
17	a	68.80	0.11844	YES	YES
18	a	69.52	0.21046	YES	YES
19	a	72.69	0.07810	YES	YES
20	a	77.62	0.18428	YES	YES
21	a	80.73	0.98281	YES	YES
22	a	84.26	0.52122	YES	YES
23	a	91.13	1.06434	YES	YES
24	a	100.44	0.18984	YES	YES
25	a	105.56	0.03076	YES	YES
26	a	111.89	0.65775	YES	YES
27	a	134.00	3.67250	YES	YES
28	a	149.45	2.90795	YES	YES
29	a	157.01	0.98042	YES	YES
30	a	158.04	0.71752	YES	YES
31	a	160.37	0.26109	YES	YES
32	a	163.86	1.50764	YES	YES
33	a	167.81	1.39280	YES	YES
34	a	185.61	6.76749	YES	YES
35	a	189.15	14.18787	YES	YES
36	a	201.55	84.48988	YES	YES
37	a	216.13	0.05430	YES	YES
38	a	262.90	1.63178	YES	YES
39	a	270.43	1.33662	YES	YES
40	a	273.95	4.58204	YES	YES
41	a	282.31	4.58849	YES	YES
42	a	286.57	4.41126	YES	YES
43	a	287.54	4.44991	YES	YES
44	a	288.88	2.26266	YES	YES
45	a	298.02	1.12358	YES	YES
46	a	300.98	9.63116	YES	YES
47	a	303.93	26.23269	YES	YES
48	a	309.09	7.88539	YES	YES
49	a	314.35	0.35443	YES	YES
50	a	317.11	3.23322	YES	YES
51	a	318.86	2.64807	YES	YES
52	a	323.53	4.29782	YES	YES
53	a	327.37	0.10371	YES	YES
54	a	336.68	4.49508	YES	YES
55	a	339.31	6.61955	YES	YES
56	a	346.09	4.83557	YES	YES
57	a	355.01	7.72268	YES	YES
58	a	370.08	4.22895	YES	YES
59	a	374.27	13.90899	YES	YES
60	a	398.87	40.73019	YES	YES
61	a	437.25	29.35345	YES	YES
62	a	469.78	2.29656	YES	YES
63	a	478.35	1.23988	YES	YES
64	a	503.31	3.32776	YES	YES
65	a	506.31	11.27233	YES	YES
66	a	517.24	4.18708	YES	YES
67	a	517.92	4.95540	YES	YES
68	a	519.52	6.72699	YES	YES
69	a	521.85	5.14343	YES	YES
70	a	523.08	4.43452	YES	YES
71	a	523.62	0.42711	YES	YES
72	a	524.47	2.60687	YES	YES
73	a	534.38	0.51317	YES	YES
74	a	550.30	2.75067	YES	YES
75	a	551.31	1.65621	YES	YES
76	a	551.74	1.28750	YES	YES

77	a	552.48	0.54467	YES	YES
78	a	556.21	0.44176	YES	YES
79	a	558.00	0.59992	YES	YES
80	a	589.28	45.97269	YES	YES
81	a	599.84	30.08031	YES	YES
82	a	696.72	28.93751	YES	YES
83	a	699.40	36.45360	YES	YES
84	a	709.59	26.35324	YES	YES
85	a	710.01	44.99987	YES	YES
86	a	711.00	7.21128	YES	YES
87	a	712.48	48.14362	YES	YES
88	a	715.07	13.15249	YES	YES
89	a	733.84	6.37311	YES	YES
90	a	742.37	1.74419	YES	YES
91	a	777.28	3.71545	YES	YES
92	a	841.81	43.91714	YES	YES
93	a	886.43	41.76263	YES	YES
94	a	898.85	183.34495	YES	YES
95	a	908.85	257.72416	YES	YES
96	a	965.74	41.95901	YES	YES
97	a	968.56	148.65967	YES	YES
98	a	973.04	148.04430	YES	YES
99	a	974.64	240.33178	YES	YES
100	a	1037.74	32.40430	YES	YES
101	a	1041.35	60.59019	YES	YES
102	a	1112.79	1.77803	YES	YES
103	a	1145.17	8.26021	YES	YES
104	a	1147.75	26.69725	YES	YES
105	a	1162.63	14.95109	YES	YES
106	a	1168.85	13.37115	YES	YES
107	a	1170.12	48.34172	YES	YES
108	a	1175.47	26.29459	YES	YES
109	a	1180.37	254.40191	YES	YES
110	a	1187.12	87.04953	YES	YES
111	a	1192.32	7.12146	YES	YES
112	a	1207.87	31.72917	YES	YES
113	a	1209.76	84.25203	YES	YES
114	a	1212.97	104.22947	YES	YES
115	a	1220.54	38.48747	YES	YES
116	a	1225.27	463.07821	YES	YES
117	a	1227.04	499.95735	YES	YES
118	a	1229.83	689.11932	YES	YES
119	a	1232.46	490.27255	YES	YES
120	a	1250.86	179.97956	YES	YES
121	a	1261.58	212.68587	YES	YES
122	a	1267.48	450.93618	YES	YES
123	a	1273.76	750.65087	YES	YES
124	a	1277.08	357.29171	YES	YES
125	a	1295.24	890.14957	YES	YES
126	a	1302.93	138.56926	YES	YES
127	a	1307.70	33.70449	YES	YES
128	a	1310.69	72.94746	YES	YES
129	a	1341.65	154.95407	YES	YES

$end

$[FAl(OC(CF_3)_3)_3]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

Al	0.1055806	0.2890985	0.9467735
O	1.6023727	-0.3183359	0.2194923
O	-0.4469427	1.6283665	-0.0711507
O	-1.1101903	-0.9864229	0.7599167
C	-1.2666975	-2.3233970	0.8184354
C	2.8024946	0.0674768	-0.2559529
C	-1.5417420	2.2829451	-0.5007881

```
C    -0.6688132   -3.0157181   -0.4676358
F     0.6719424   -3.1288669   -0.3817837
F    -0.9525322   -2.2904701   -1.5584630
F    -1.1685268   -4.2657023   -0.6568436
C    -0.5710921   -2.9240118    2.0956816
F    -0.4395507   -4.2714491    2.0380249
F    -1.2765243   -2.6305194    3.2092409
F     0.6565180   -2.3958407    2.2440602
C    -2.8118957   -2.6202290    0.8872443
F    -3.3891817   -2.4403438   -0.3202019
F    -3.4113295   -1.7906635    1.7536731
F    -3.0797449   -3.8926027    1.2777908
C     2.8620043    1.6198231   -0.5245248
F     2.1861081    1.9420184   -1.6446812
F     4.1312050    2.0766051   -0.6683670
F     2.3038978    2.2844827    0.5022143
C     3.9216825   -0.3166080    0.7859131
F     5.1683758   -0.2862152    0.2494195
F     3.7126429   -1.5510539    1.2677207
F     3.9094441    0.5359254    1.8340515
C     3.0685763   -0.6938741   -1.6088299
F     1.9739197   -0.6727587   -2.3812613
F     3.3850532   -1.9872932   -1.3809248
F     4.0906583   -0.1465707   -2.3159976
C    -2.4007274    2.8030124    0.7101678
F    -3.6325195    3.2259856    0.3334260
F    -1.7854909    3.8358770    1.3250791
F    -2.5605524    1.8277726    1.6214457
C    -1.0486242    3.5128117   -1.3528767
F    -2.0259716    4.4308812   -1.5608519
F    -0.6087113    3.1062823   -2.5631746
F    -0.0321275    4.1343847   -0.7374608
C    -2.4461252    1.3618479   -1.4116122
F    -1.6808871    0.5900933   -2.1946027
F    -3.2665618    2.0887969   -2.2158145
F    -3.2305082    0.5564407   -0.6685149
F     0.3010942    0.7480191    2.5625430

SCF energy GEOOPT =  -3718.967219020 H
ZPE =   437.2 kJ/mol
FREEH energy =   550.66 kJ/mol
FREEH entropy =   1.11408 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a              9.48         0.05205       YES     YES
     8        a             14.49         0.01647       YES     YES
     9        a             15.63         0.01512       YES     YES
    10        a             20.48         0.07925       YES     YES
    11        a             25.37         0.15364       YES     YES
    12        a             26.21         0.14203       YES     YES
    13        a             33.00         0.08475       YES     YES
    14        a             40.61         0.11139       YES     YES
    15        a             60.71         0.05379       YES     YES
    16        a             67.85         0.46825       YES     YES
    17        a             69.01         0.05409       YES     YES
    18        a             71.75         0.21917       YES     YES
    19        a             74.41         0.01367       YES     YES
    20        a             76.94         0.08453       YES     YES
    21        a             77.68         0.17367       YES     YES
    22        a             81.25         0.03055       YES     YES
    23        a             85.60         0.03370       YES     YES
    24        a             86.25         0.07268       YES     YES
```

25	a	88.80	0.04636	YES	YES
26	a	91.47	0.36868	YES	YES
27	a	98.36	0.27424	YES	YES
28	a	129.57	3.31693	YES	YES
29	a	133.09	1.92552	YES	YES
30	a	151.52	0.20064	YES	YES
31	a	158.40	0.18707	YES	YES
32	a	158.58	0.24509	YES	YES
33	a	163.62	0.25719	YES	YES
34	a	165.31	1.90315	YES	YES
35	a	167.74	2.20333	YES	YES
36	a	189.41	0.49618	YES	YES
37	a	193.00	7.01740	YES	YES
38	a	195.93	7.41938	YES	YES
39	a	232.09	0.15638	YES	YES
40	a	268.85	2.10425	YES	YES
41	a	270.47	1.14315	YES	YES
42	a	277.07	4.02804	YES	YES
43	a	279.01	3.19555	YES	YES
44	a	279.43	3.45075	YES	YES
45	a	284.09	0.17600	YES	YES
46	a	284.57	0.25245	YES	YES
47	a	286.19	0.38950	YES	YES
48	a	290.15	4.45213	YES	YES
49	a	304.41	10.99296	YES	YES
50	a	305.11	10.91796	YES	YES
51	a	309.56	0.04217	YES	YES
52	a	317.03	0.14326	YES	YES
53	a	317.52	0.58913	YES	YES
54	a	321.25	2.44534	YES	YES
55	a	321.77	2.51128	YES	YES
56	a	323.40	2.45991	YES	YES
57	a	328.10	0.23183	YES	YES
58	a	349.06	2.50591	YES	YES
59	a	351.00	1.89179	YES	YES
60	a	359.23	28.92916	YES	YES
61	a	360.46	25.10890	YES	YES
62	a	368.16	12.60013	YES	YES
63	a	409.81	5.15165	YES	YES
64	a	450.47	63.73450	YES	YES
65	a	451.92	59.60032	YES	YES
66	a	516.95	0.48205	YES	YES
67	a	517.27	4.39321	YES	YES
68	a	518.17	3.85284	YES	YES
69	a	518.49	4.10862	YES	YES
70	a	520.18	8.62365	YES	YES
71	a	520.24	6.09350	YES	YES
72	a	521.28	2.98186	YES	YES
73	a	523.88	3.35927	YES	YES
74	a	524.33	2.49132	YES	YES
75	a	527.90	0.24115	YES	YES
76	a	548.35	24.53433	YES	YES
77	a	548.77	19.43989	YES	YES
78	a	553.68	0.52551	YES	YES
79	a	553.95	0.91591	YES	YES
80	a	554.14	0.31985	YES	YES
81	a	555.09	2.21814	YES	YES
82	a	558.72	18.86334	YES	YES
83	a	560.67	25.03372	YES	YES
84	a	706.32	4.64054	YES	YES
85	a	706.55	9.02028	YES	YES
86	a	707.37	18.67767	YES	YES
87	a	708.22	44.44661	YES	YES
88	a	708.65	82.45717	YES	YES
89	a	710.00	47.36226	YES	YES
90	a	716.25	4.01567	YES	YES
91	a	735.33	6.46289	YES	YES
92	a	736.01	6.82033	YES	YES
93	a	758.91	12.35613	YES	YES
94	a	811.75	31.78199	YES	YES

95	a	813.28	32.83532	YES	YES
96	a	842.88	57.58444	YES	YES
97	a	956.70	30.00985	YES	YES
98	a	957.85	51.57530	YES	YES
99	a	958.49	38.50296	YES	YES
100	a	963.34	325.03808	YES	YES
101	a	964.76	190.27993	YES	YES
102	a	966.27	213.16826	YES	YES
103	a	1110.55	11.65094	YES	YES
104	a	1111.95	12.15471	YES	YES
105	a	1116.63	4.07995	YES	YES
106	a	1128.53	8.79433	YES	YES
107	a	1129.94	18.71550	YES	YES
108	a	1132.89	9.97972	YES	YES
109	a	1134.76	23.85545	YES	YES
110	a	1138.69	2.30257	YES	YES
111	a	1139.37	10.68601	YES	YES
112	a	1195.96	18.09948	YES	YES
113	a	1199.38	64.47928	YES	YES
114	a	1202.12	35.62494	YES	YES
115	a	1204.71	41.65706	YES	YES
116	a	1207.63	38.45490	YES	YES
117	a	1213.70	89.36393	YES	YES
118	a	1217.00	994.24469	YES	YES
119	a	1218.97	950.28415	YES	YES
120	a	1231.61	443.44696	YES	YES
121	a	1234.29	359.62093	YES	YES
122	a	1236.15	28.36531	YES	YES
123	a	1238.78	202.22982	YES	YES
124	a	1246.45	18.53035	YES	YES
125	a	1249.84	49.45155	YES	YES
126	a	1252.60	195.69219	YES	YES
127	a	1255.88	524.12860	YES	YES
128	a	1258.87	682.66988	YES	YES
129	a	1266.15	964.42581	YES	YES
130	a	1338.10	244.42498	YES	YES
131	a	1340.84	269.14043	YES	YES
132	a	1357.90	52.17836	YES	YES

$end

$Al(C_6F_5)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C    -0.7758424   -4.1954753   -0.3362496
C    -0.8643148   -2.7986382   -0.4328101
C     0.1898426   -1.9449093   -0.0665943
C     1.3675635   -2.5563631    0.3952585
C     1.5042902   -3.9485773    0.5088748
C     0.4206244   -4.7666803    0.1378930
F    -2.0138834   -2.2810032   -0.9078017
F    -1.7951738   -4.9829932   -0.6895948
F     0.5272208   -6.0907783    0.2366827
F     2.6325992   -4.5012791    0.9627222
F     2.4159663   -1.7978973    0.7710376
C    -2.1332202    1.9268715   -0.7466861
C    -3.9977645    0.8792226    1.0547199
C    -1.7689260    0.8102238    0.0174994
C    -2.7250780    0.3079841    0.9107306
C    -4.3241339    2.0029001    0.2714945
C    -3.3926655    2.5370402   -0.6389355
F    -1.2539857    2.4411608   -1.6320258
F    -4.8905847    0.3894816    1.9190123
F    -3.7199810    3.6003754   -1.3784299
F    -5.5255637    2.5660300    0.3951227
F    -2.4157675   -0.7540196    1.6843204
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C     2.5813823    0.9683513   -1.1586318
C     2.9174394    2.9732166    0.7627632
C     1.5842372    1.1424632   -0.1920112
C     1.7791196    2.1529410    0.7570764
C     3.8992532    2.7665086   -0.2249466
C     3.7382782    1.7609555   -1.1980138
F     2.4287342    0.0112683   -2.0986334
F     3.0892499    3.9258552    1.6833098
F     4.6771233    1.5838999   -2.1315591
F     4.9913136    3.5302986   -0.2394217
F     0.8500243    2.3423166    1.7196252
Al    0.0026231   -0.0007509   -0.1157977

SCF energy GEOOPT =  -2424.394495507 H
ZPE =   381.1 kJ/mol
FREEH energy =   463.17 kJ/mol
FREEH entropy =   0.87140 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             11.66         0.01630       YES     YES
     8        a             16.28         0.03095       YES     YES
     9        a             21.47         0.15316       YES     YES
    10        a             22.54         0.18496       YES     YES
    11        a             26.69         0.17277       YES     YES
    12        a             27.26         0.00510       YES     YES
    13        a             66.06         0.00573       YES     YES
    14        a             74.62         0.01489       YES     YES
    15        a             80.43         0.07546       YES     YES
    16        a            100.72         0.65822       YES     YES
    17        a            102.88         0.55922       YES     YES
    18        a            122.69         0.02408       YES     YES
    19        a            124.83         0.01607       YES     YES
    20        a            125.16         0.01478       YES     YES
    21        a            129.93         0.02376       YES     YES
    22        a            142.76         0.27625       YES     YES
    23        a            147.30         0.05439       YES     YES
    24        a            150.50         0.06393       YES     YES
    25        a            201.74         6.34192       YES     YES
    26        a            211.94         0.61397       YES     YES
    27        a            216.54         0.69387       YES     YES
    28        a            234.62         6.01917       YES     YES
    29        a            262.16         1.28000       YES     YES
    30        a            262.98         1.12977       YES     YES
    31        a            263.91         1.63488       YES     YES
    32        a            264.69         0.33720       YES     YES
    33        a            265.56         0.02678       YES     YES
    34        a            267.45         0.02947       YES     YES
    35        a            303.17         2.13290       YES     YES
    36        a            304.33         2.59338       YES     YES
    37        a            304.72         0.55235       YES     YES
    38        a            319.74        20.29951       YES     YES
    39        a            319.94        20.67880       YES     YES
    40        a            342.32         0.04376       YES     YES
    41        a            350.84         0.70103       YES     YES
    42        a            354.81         0.46132       YES     YES
    43        a            364.93        10.63609       YES     YES
    44        a            400.94         0.74754       YES     YES
    45        a            404.34        40.38337       YES     YES
    46        a            404.69        13.00581       YES     YES
    47        a            405.18        56.05398       YES     YES
    48        a            407.15         1.62338       YES     YES
    49        a            431.46         0.24374       YES     YES
```

50	a	431.96	0.53757	YES	YES
51	a	432.19	0.46967	YES	YES
52	a	456.64	1.92277	YES	YES
53	a	465.86	2.35473	YES	YES
54	a	478.82	1.63085	YES	YES
55	a	480.79	0.11948	YES	YES
56	a	509.94	46.07161	YES	YES
57	a	511.12	44.03690	YES	YES
58	a	564.61	0.64173	YES	YES
59	a	565.68	1.07386	YES	YES
60	a	566.28	1.66099	YES	YES
61	a	601.35	3.81267	YES	YES
62	a	605.65	6.33259	YES	YES
63	a	609.77	12.23964	YES	YES
64	a	630.14	0.01674	YES	YES
65	a	631.42	0.07651	YES	YES
66	a	632.45	0.09138	YES	YES
67	a	737.59	2.39670	YES	YES
68	a	741.98	6.41333	YES	YES
69	a	742.92	7.05053	YES	YES
70	a	797.61	0.19410	YES	YES
71	a	836.16	1.30143	YES	YES
72	a	838.13	0.47615	YES	YES
73	a	971.69	184.64945	YES	YES
74	a	973.19	96.23944	YES	YES
75	a	975.92	142.76609	YES	YES
76	a	1092.44	46.06213	YES	YES
77	a	1094.88	376.92018	YES	YES
78	a	1097.01	354.02323	YES	YES
79	a	1151.36	3.43085	YES	YES
80	a	1153.15	0.65161	YES	YES
81	a	1154.60	1.76941	YES	YES
82	a	1287.82	66.91235	YES	YES
83	a	1288.93	51.10668	YES	YES
84	a	1291.62	44.91284	YES	YES
85	a	1357.16	1.28042	YES	YES
86	a	1362.41	1.69849	YES	YES
87	a	1364.04	2.70739	YES	YES
88	a	1370.49	93.56204	YES	YES
89	a	1376.07	104.34381	YES	YES
90	a	1385.86	6.24718	YES	YES
91	a	1472.57	515.32051	YES	YES
92	a	1481.14	455.18759	YES	YES
93	a	1484.02	615.38861	YES	YES
94	a	1516.42	299.54248	YES	YES
95	a	1517.46	291.66845	YES	YES
96	a	1519.65	10.62554	YES	YES
97	a	1612.75	6.07446	YES	YES
98	a	1618.36	4.64393	YES	YES
99	a	1619.67	5.46400	YES	YES
100	a	1626.49	103.82149	YES	YES
101	a	1629.98	83.52163	YES	YES
102	a	1631.47	52.57702	YES	YES

$end

$[FAl(C_6F_5)_3]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

C	-0.7105892	-3.9779568	-0.5574127
C	-0.8538338	-2.6521664	-0.1082021
C	0.1756158	-1.9403970	0.5142123
C	1.3775851	-2.6356894	0.6865009
C	1.5784663	-3.9588460	0.2623395
C	0.5161221	-4.6321367	-0.3642698
F	-2.0624286	-2.0815872	-0.3238112

```
F    -1.7227149   -4.6297019   -1.1622143
F     0.6748438   -5.9012603   -0.7819595
F     2.7541620   -4.5914906    0.4417433
F     2.4266956   -2.0230091    1.2843018
C    -1.7648301    1.6308499   -0.6085916
C    -4.0939280    1.0616744    0.8003230
C    -1.6502778    0.8198604    0.5250908
C    -2.8458005    0.5589780    1.2041782
C    -4.1573844    1.8739761   -0.3438372
C    -2.9855919    2.1635712   -1.0598810
F    -0.6780979    1.9330268   -1.3591021
F    -5.2228430    0.7807789    1.4800665
F    -3.0500037    2.9382950   -2.1603487
F    -5.3388709    2.3660351   -0.7577439
F    -2.8433475   -0.2352378    2.2981551
C     2.3748764    0.6808396   -0.7594963
C     2.7639299    3.2321042    0.2840555
C     1.5854275    1.0615084    0.3290308
C     1.8039949    2.3545472    0.8144134
C     3.5404635    2.8014516   -0.8034908
C     3.3490859    1.5158234   -1.3350302
F     2.2115872   -0.5317313   -1.3408223
F     2.9452983    4.4702114    0.7833086
F     4.0896544    1.1178282   -2.3882020
F     4.4641975    3.6213592   -1.3373632
F     1.0528775    2.8267775    1.8380918
Al    0.0849594   -0.0207288    1.1509274
F     0.2106989    0.0024426    2.8550398

SCF energy GEOOPT =  -2524.355561048 H
ZPE =   383.4 kJ/mol
FREEH energy =   469.38 kJ/mol
FREEH entropy =   0.89970 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a              7.07         0.00506       YES     YES
     8        a             12.74         0.02235       YES     YES
     9        a             21.85         0.01384       YES     YES
    10        a             25.29         0.01829       YES     YES
    11        a             25.72         0.02255       YES     YES
    12        a             29.95         0.04388       YES     YES
    13        a             72.80         0.97892       YES     YES
    14        a             78.94         0.15644       YES     YES
    15        a             86.24         0.48609       YES     YES
    16        a            100.68         0.01644       YES     YES
    17        a            103.27         0.02205       YES     YES
    18        a            110.93         0.14999       YES     YES
    19        a            120.38         0.02293       YES     YES
    20        a            122.12         0.02435       YES     YES
    21        a            124.42         0.12569       YES     YES
    22        a            140.77         5.47100       YES     YES
    23        a            149.38         2.91202       YES     YES
    24        a            153.09         0.17258       YES     YES
    25        a            156.89         1.43982       YES     YES
    26        a            159.37         1.71145       YES     YES
    27        a            209.86         1.47956       YES     YES
    28        a            215.95         0.51336       YES     YES
    29        a            218.14         0.57238       YES     YES
    30        a            235.84         0.14825       YES     YES
    31        a            261.85         0.11366       YES     YES
    32        a            262.34         0.15948       YES     YES
    33        a            262.74         0.05714       YES     YES
```

34	a	266.05	0.74334	YES	YES
35	a	266.61	0.47375	YES	YES
36	a	268.38	0.24820	YES	YES
37	a	302.84	3.73144	YES	YES
38	a	303.68	4.12757	YES	YES
39	a	305.18	1.06103	YES	YES
40	a	321.79	29.05928	YES	YES
41	a	324.08	25.97717	YES	YES
42	a	342.79	0.75907	YES	YES
43	a	348.01	0.22740	YES	YES
44	a	352.32	0.68004	YES	YES
45	a	364.89	2.76068	YES	YES
46	a	394.30	59.91137	YES	YES
47	a	396.84	54.70324	YES	YES
48	a	398.47	20.99996	YES	YES
49	a	400.61	6.54975	YES	YES
50	a	400.88	8.89859	YES	YES
51	a	433.04	0.14251	YES	YES
52	a	433.88	0.85592	YES	YES
53	a	434.20	0.98336	YES	YES
54	a	459.95	2.76352	YES	YES
55	a	469.54	0.94638	YES	YES
56	a	472.09	2.20567	YES	YES
57	a	475.96	0.21752	YES	YES
58	a	489.03	38.68575	YES	YES
59	a	490.08	44.02103	YES	YES
60	a	562.46	0.06138	YES	YES
61	a	562.69	0.17730	YES	YES
62	a	563.88	0.11781	YES	YES
63	a	593.92	8.36987	YES	YES
64	a	594.60	8.32325	YES	YES
65	a	599.59	17.85830	YES	YES
66	a	630.39	0.08180	YES	YES
67	a	633.11	0.49950	YES	YES
68	a	633.93	0.23950	YES	YES
69	a	727.89	5.70085	YES	YES
70	a	732.92	3.94686	YES	YES
71	a	734.59	4.28318	YES	YES
72	a	751.10	47.35980	YES	YES
73	a	785.79	0.96626	YES	YES
74	a	787.23	0.83403	YES	YES
75	a	796.98	29.18257	YES	YES
76	a	959.98	188.97202	YES	YES
77	a	962.68	104.70472	YES	YES
78	a	964.04	208.32019	YES	YES
79	a	1069.16	377.82298	YES	YES
80	a	1069.96	250.67664	YES	YES
81	a	1072.30	160.71189	YES	YES
82	a	1124.93	1.28077	YES	YES
83	a	1127.07	0.18359	YES	YES
84	a	1128.97	0.78851	YES	YES
85	a	1252.74	58.99819	YES	YES
86	a	1253.74	39.44213	YES	YES
87	a	1256.19	29.33173	YES	YES
88	a	1355.84	27.29110	YES	YES
89	a	1358.14	28.27745	YES	YES
90	a	1360.75	2.35760	YES	YES
91	a	1364.76	14.20039	YES	YES
92	a	1366.17	11.17531	YES	YES
93	a	1371.06	1.08493	YES	YES
94	a	1454.27	477.86548	YES	YES
95	a	1457.55	407.77326	YES	YES
96	a	1462.41	633.83379	YES	YES
97	a	1504.27	207.59585	YES	YES
98	a	1504.84	174.06529	YES	YES
99	a	1506.94	36.88021	YES	YES
100	a	1616.41	3.76849	YES	YES
101	a	1617.10	8.02694	YES	YES
102	a	1618.65	4.57282	YES	YES
103	a	1620.66	65.20987	YES	YES

```
   104        a            1620.81        70.88614       YES     YES
   105        a            1621.30        18.15589       YES     YES
$end
```

$Al(OTeF_5)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Te        -2.96170       -0.33183       -0.01686
O         -1.38278       -1.32298        0.31712
F         -1.45742        1.05960       -0.46774
F         -4.20976        1.04532       -0.47216
F         -4.29198       -1.62209        0.42761
F         -3.06210       -0.79663       -1.87975
F         -3.04031        0.41791        1.75367
Te         1.50004        0.62404       -2.52816
O          0.30751       -0.67245       -1.82976
F          1.78550       -0.04084       -4.29148
F          2.62397        2.15635       -2.74830
F          1.17088        1.32505       -0.58186
F          0.09232        1.78006       -3.14836
F          3.09346       -0.24943       -1.89833
Te         1.48308       -0.55829        2.49030
O          1.35469       -1.18601        0.70722
F          2.82037       -1.71974        3.19503
F          1.25477        0.43854        4.10749
F          0.01535        0.70080        1.68391
F          2.81119        0.76641        2.06223
F          0.08230       -1.68102        3.18065
Al         0.01064       -0.13280       -0.06246

SCF energy GEOOPT =  -1988.876604356 H
ZPE =   124.7 kJ/mol
FREEH energy =   199.43 kJ/mol
FREEH entropy =   0.79318 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             26.74         0.08741       YES     YES
     8        a             28.33         0.06028       YES     YES
     9        a             45.55         0.11642       YES     YES
    10        a             55.09         0.00541       YES     YES
    11        a             56.91         0.08049       YES     YES
    12        a             61.04         0.01675       YES     YES
    13        a            100.67         0.60961       YES     YES
    14        a            106.71         0.44349       YES     YES
    15        a            107.96         0.01419       YES     YES
    16        a            109.08         0.20367       YES     YES
    17        a            110.41         0.08029       YES     YES
    18        a            112.48         0.07611       YES     YES
    19        a            147.05         0.00750       YES     YES
    20        a            159.61         2.47084       YES     YES
    21        a            162.68         4.52475       YES     YES
    22        a            173.86         2.41201       YES     YES
    23        a            179.69         0.78682       YES     YES
    24        a            184.48         0.57165       YES     YES
    25        a            205.01         7.27180       YES     YES
    26        a            206.34        14.92176       YES     YES
    27        a            208.01        10.76865       YES     YES
```

28	a	226.37	27.91901	YES	YES
29	a	237.23	4.41369	YES	YES
30	a	239.28	2.67860	YES	YES
31	a	240.86	4.87893	YES	YES
32	a	252.70	36.68990	YES	YES
33	a	254.71	37.98603	YES	YES
34	a	278.97	1.51614	YES	YES
35	a	288.40	21.56938	YES	YES
36	a	288.68	17.23443	YES	YES
37	a	290.17	15.29123	YES	YES
38	a	298.10	9.85314	YES	YES
39	a	303.17	108.21218	YES	YES
40	a	304.92	109.25170	YES	YES
41	a	338.69	19.43526	YES	YES
42	a	340.96	15.37102	YES	YES
43	a	382.56	7.05923	YES	YES
44	a	383.61	6.71723	YES	YES
45	a	410.53	1.78207	YES	YES
46	a	487.71	32.73544	YES	YES
47	a	488.60	30.95242	YES	YES
48	a	521.62	32.12567	YES	YES
49	a	581.50	71.81814	YES	YES
50	a	581.96	67.31155	YES	YES
51	a	584.88	5.94106	YES	YES
52	a	604.95	15.29377	YES	YES
53	a	607.57	62.26477	YES	YES
54	a	608.20	61.70786	YES	YES
55	a	619.78	15.87758	YES	YES
56	a	633.01	43.61919	YES	YES
57	a	635.67	45.68210	YES	YES
58	a	645.02	8.78786	YES	YES
59	a	647.57	58.36522	YES	YES
60	a	648.60	71.56666	YES	YES
61	a	655.72	200.87505	YES	YES
62	a	656.16	136.32537	YES	YES
63	a	656.51	188.91936	YES	YES
64	a	683.91	221.93418	YES	YES
65	a	685.27	214.22094	YES	YES
66	a	703.32	5.01684	YES	YES

$end

$[FAl(OTeF_5)_3]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

Al	-0.36886	0.75109	0.89079
O	1.38708	0.59913	1.26308
O	-0.44464	0.53949	-0.89303
O	-1.11843	-0.65402	1.73383
Te	2.79705	1.32553	0.23452
Te	-0.63542	-2.46579	1.47794
Te	-1.97100	0.75825	-1.98084
F	0.66959	-2.10428	0.09806
F	-0.18181	-4.32974	1.26572
F	-1.97726	-2.77574	0.12894
F	-1.89278	-3.02348	2.82469
F	0.75215	-2.42565	2.81636
F	2.58702	0.12313	-1.25500
F	4.07099	0.12613	1.03427
F	4.27160	2.07321	-0.76136
F	3.23373	2.63350	1.58527
F	1.67526	2.63807	-0.64276
F	-3.19567	0.50632	-0.49949
F	-2.08512	-1.11523	-2.40883
F	-3.53034	0.96937	-3.09805
F	-0.90400	1.02455	-3.55808

```
F         -2.07085        2.67039       -1.73629
F         -1.06828        2.15578        1.48025

SCF energy GEOOPT =  -2088.841335504 H
ZPE =   128.9 kJ/mol
FREEH energy =   209.76 kJ/mol
FREEH entropy =   0.86464 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000         -       -
     2                      -0.00         0.00000         -       -
     3                      -0.00         0.00000         -       -
     4                      -0.00         0.00000         -       -
     5                      -0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
     7        a             15.50         0.05898       YES     YES
     8        a             22.78         0.00426       YES     YES
     9        a             28.41         0.03243       YES     YES
    10        a             33.56         0.04188       YES     YES
    11        a             36.22         0.00704       YES     YES
    12        a             43.98         0.07427       YES     YES
    13        a             55.80         0.21750       YES     YES
    14        a             60.19         0.01660       YES     YES
    15        a             70.41         0.03304       YES     YES
    16        a             86.83         0.28721       YES     YES
    17        a             90.80         1.99097       YES     YES
    18        a            100.08         1.13908       YES     YES
    19        a            128.42         4.29656       YES     YES
    20        a            135.73         2.80031       YES     YES
    21        a            164.62         2.23581       YES     YES
    22        a            168.16         2.83027       YES     YES
    23        a            169.57         0.49550       YES     YES
    24        a            171.70         1.07040       YES     YES
    25        a            173.53         3.27544       YES     YES
    26        a            176.00         1.17296       YES     YES
    27        a            185.02         6.08264       YES     YES
    28        a            190.25         5.79747       YES     YES
    29        a            191.54        10.47721       YES     YES
    30        a            224.31         0.92467       YES     YES
    31        a            246.24         1.39768       YES     YES
    32        a            248.47         0.07391       YES     YES
    33        a            250.23         1.22402       YES     YES
    34        a            262.02         4.03346       YES     YES
    35        a            266.59        76.88833       YES     YES
    36        a            271.60        94.92000       YES     YES
    37        a            275.73         8.47042       YES     YES
    38        a            277.60         7.44623       YES     YES
    39        a            277.99        40.67550       YES     YES
    40        a            282.43        31.56055       YES     YES
    41        a            283.77         7.89208       YES     YES
    42        a            285.87        24.88497       YES     YES
    43        a            291.03       109.48011       YES     YES
    44        a            298.13        16.18702       YES     YES
    45        a            303.42        49.33996       YES     YES
    46        a            328.69        16.71791       YES     YES
    47        a            349.61        19.42418       YES     YES
    48        a            466.03        11.47726       YES     YES
    49        a            534.85        55.67489       YES     YES
    50        a            542.28        50.63993       YES     YES
    51        a            579.15         1.83088       YES     YES
    52        a            581.41         5.75697       YES     YES
    53        a            583.93         0.42643       YES     YES
    54        a            584.62         0.79402       YES     YES
    55        a            585.79         3.41322       YES     YES
    56        a            587.24         8.54911       YES     YES
    57        a            610.89        27.85820       YES     YES
    58        a            618.26        65.33387       YES     YES
    59        a            620.86        82.70762       YES     YES
```

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    60        a             637.89        17.22786       YES     YES
    61        a             641.36        79.54829       YES     YES
    62        a             643.35         7.79305       YES     YES
    63        a             645.34       142.36607       YES     YES
    64        a             647.84        96.62461       YES     YES
    65        a             649.44       231.24653       YES     YES
    66        a             789.22        13.28855       YES     YES
    67        a             794.93       425.04834       YES     YES
    68        a             804.87       377.97728       YES     YES
    69        a             873.76       156.64359       YES     YES
$end
```

$Ga(OTeF_5)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Ga        -0.02579       -0.26483       -0.24905
O          1.59979       -1.11120       -0.79206
O         -0.73470        0.36475       -1.91013
O         -1.16715       -1.74970        0.14605
Te         2.93201        0.25392       -0.70668
Te        -0.93613       -2.07421        2.01276
Te        -2.01591        1.69930       -1.44013
F          0.60169       -3.20316        1.77364
F         -0.46486       -2.06997        3.86609
F         -2.08002       -3.59099        2.18006
F         -2.35704       -0.88372        2.52321
F          0.30240       -0.44757        1.81369
F          2.53186        0.95799       -2.45068
F          4.39622       -0.75443       -1.39680
F          3.97638        1.83830       -0.46545
F          3.43252       -0.16985        1.10024
F          1.33810        1.31906        0.02135
F         -0.73097        3.12788       -1.49690
F         -1.34667        1.21593        0.44029
F         -3.16330        2.96711       -0.58173
F         -3.45840        0.45183       -1.19221
F         -2.63001        2.12357       -3.19555

SCF energy GEOOPT =  -3671.288067594 H
ZPE =   120.1 kJ/mol
FREEH energy =   197.06 kJ/mol
FREEH entropy =   0.81575 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             21.65         0.14781       YES     YES
     8        a             27.36         0.25132       YES     YES
     9        a             47.11         0.06609       YES     YES
    10        a             50.22         0.08008       YES     YES
    11        a             53.15         0.00148       YES     YES
    12        a             58.52         0.00613       YES     YES
    13        a             89.80         0.48944       YES     YES
    14        a             93.71         0.27679       YES     YES
    15        a             96.62         0.51320       YES     YES
    16        a            102.26         2.46919       YES     YES
    17        a            104.61         1.79499       YES     YES
    18        a            110.48         0.44341       YES     YES
    19        a            123.10         0.10427       YES     YES
```

```
    20        a             157.73        11.95178       YES     YES
    21        a             160.44        14.66140       YES     YES
    22        a             173.03         2.27010       YES     YES
    23        a             174.58         0.84566       YES     YES
    24        a             176.43         0.33271       YES     YES
    25        a             189.63         0.81528       YES     YES
    26        a             191.02        18.04825       YES     YES
    27        a             192.41        19.90049       YES     YES
    28        a             208.32        12.83891       YES     YES
    29        a             228.05        22.80058       YES     YES
    30        a             230.19        22.05428       YES     YES
    31        a             240.47         0.70587       YES     YES
    32        a             242.55         4.51070       YES     YES
    33        a             244.00         4.79575       YES     YES
    34        a             277.32         0.47792       YES     YES
    35        a             282.47        33.22066       YES     YES
    36        a             283.30        19.70231       YES     YES
    37        a             285.03        10.45191       YES     YES
    38        a             286.35        17.99713       YES     YES
    39        a             289.57        38.98300       YES     YES
    40        a             290.89        24.22605       YES     YES
    41        a             298.00        99.62048       YES     YES
    42        a             300.60        91.17556       YES     YES
    43        a             319.83         0.49914       YES     YES
    44        a             320.99         1.05181       YES     YES
    45        a             353.47        29.51230       YES     YES
    46        a             486.73        52.50911       YES     YES
    47        a             488.37        49.88026       YES     YES
    48        a             511.84        32.00402       YES     YES
    49        a             546.22       120.61612       YES     YES
    50        a             547.43       109.80197       YES     YES
    51        a             550.73        35.14592       YES     YES
    52        a             591.73         1.52585       YES     YES
    53        a             592.28         1.53161       YES     YES
    54        a             592.75         1.26011       YES     YES
    55        a             616.96         4.95297       YES     YES
    56        a             618.12         4.02444       YES     YES
    57        a             620.70        13.70453       YES     YES
    58        a             646.21         2.57236       YES     YES
    59        a             647.36        34.92672       YES     YES
    60        a             647.88        34.49046       YES     YES
    61        a             651.83       113.86637       YES     YES
    62        a             652.20       108.40301       YES     YES
    63        a             652.55       152.10556       YES     YES
    64        a             666.89       274.82822       YES     YES
    65        a             667.41       263.62783       YES     YES
    66        a             700.57        17.06168       YES     YES
$end
```

$[FGa(OTeF_5)_3]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Ga        -0.70127        0.10001        0.87263
O          1.01461        0.13411        0.10945
O         -1.75327        1.47603        0.13647
O         -1.50259       -1.47516        0.21737
Te         2.41503        1.17452        0.86247
Te        -0.60656       -3.14243        0.38162
Te        -1.66066        1.92357       -1.70755
F          0.53732       -2.86968       -1.14560
F          0.26759       -4.85464        0.54560
F         -1.90056       -4.01233       -0.74767
F         -1.63644       -3.68116        1.92425
F          0.76760       -2.44692        1.56136
F          2.74691        2.11632       -0.78310
```

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F          3.75264       -0.11373        0.35503
F          3.84189        2.24568        1.59750
F          2.32736        0.35727        2.61027
F          1.20532        2.56983        1.45461
F         -3.38997        1.16311       -2.10128
F         -0.81772        0.26604       -2.24299
F         -1.61163        2.42486       -3.56924
F          0.06741        2.77350       -1.58008
F         -2.51200        3.61873       -1.37205
F         -0.85102        0.25247        2.62092

SCF energy GEOOPT =  -3771.252700518 H
ZPE =   123.9 kJ/mol
FREEH energy =   206.56 kJ/mol
FREEH entropy =   0.88166 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                       -0.00         0.00000        -       -
     2                       -0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              16.76         0.12949       YES     YES
     8        a              18.99         0.02809       YES     YES
     9        a              27.32         0.07865       YES     YES
    10        a              29.89         0.06439       YES     YES
    11        a              36.02         0.00665       YES     YES
    12        a              47.59         0.06165       YES     YES
    13        a              55.41         0.89268       YES     YES
    14        a              60.47         0.09318       YES     YES
    15        a              72.30         0.16625       YES     YES
    16        a              78.02         2.29274       YES     YES
    17        a              81.98         0.42874       YES     YES
    18        a              91.18         2.18769       YES     YES
    19        a             124.90         3.37900       YES     YES
    20        a             127.12         2.14647       YES     YES
    21        a             147.38         2.90140       YES     YES
    22        a             157.83         5.47488       YES     YES
    23        a             164.08        15.59238       YES     YES
    24        a             167.31         0.84792       YES     YES
    25        a             169.98         5.75164       YES     YES
    26        a             172.90         0.40621       YES     YES
    27        a             178.09         1.82073       YES     YES
    28        a             179.25        12.87404       YES     YES
    29        a             185.41         5.86631       YES     YES
    30        a             205.76         2.32167       YES     YES
    31        a             223.80        14.32052       YES     YES
    32        a             230.96        37.43947       YES     YES
    33        a             246.68         6.04637       YES     YES
    34        a             247.83         0.96559       YES     YES
    35        a             249.53         3.99113       YES     YES
    36        a             265.46        59.94132       YES     YES
    37        a             272.73         8.46619       YES     YES
    38        a             274.73        24.38254       YES     YES
    39        a             275.70        11.39762       YES     YES
    40        a             280.56        18.43290       YES     YES
    41        a             280.87         6.71236       YES     YES
    42        a             284.21        75.07452       YES     YES
    43        a             287.50        84.09694       YES     YES
    44        a             291.54        50.45803       YES     YES
    45        a             292.25        31.28914       YES     YES
    46        a             297.89        31.56731       YES     YES
    47        a             307.82         0.28504       YES     YES
    48        a             466.80        16.11642       YES     YES
    49        a             490.36        36.53617       YES     YES
    50        a             494.46        56.13688       YES     YES
    51        a             576.49         6.42827       YES     YES
```

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    52        a             577.39         3.77877       YES     YES
    53        a             579.79         1.26400       YES     YES
    54        a             582.32         3.12064       YES     YES
    55        a             583.47         1.35386       YES     YES
    56        a             585.24         0.25519       YES     YES
    57        a             609.13        24.77953       YES     YES
    58        a             609.52        55.69805       YES     YES
    59        a             610.56        54.77317       YES     YES
    60        a             635.98        25.22856       YES     YES
    61        a             639.42        79.35337       YES     YES
    62        a             640.61        12.80041       YES     YES
    63        a             642.37       156.94797       YES     YES
    64        a             644.75       183.92818       YES     YES
    65        a             647.04        90.58581       YES     YES
    66        a             687.09        97.54037       YES     YES
    67        a             718.21       371.46933       YES     YES
    68        a             725.29       251.33743       YES     YES
    69        a             760.04        60.10873       YES     YES
$end
```

$Al(OC_5F_4N)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c3

Cartesian coordinates in Ångström:
Al        -0.00000        0.00000        0.68126
O         -1.60138       -0.51445        1.27443
C         -2.27071       -1.45517        0.62367
C         -3.51980       -1.97918        1.02818
C         -4.09661       -2.97649        0.21914
N         -3.55063       -3.44829       -0.89097
C         -2.38651       -2.97598       -1.29742
C         -1.73512       -1.98931       -0.56645
F         -4.11637       -1.54084        2.13652
F         -0.50547       -1.43487       -0.92485
F         -1.85097       -3.46204       -2.41707
F         -5.27170       -3.48651        0.58772
O          1.24622       -1.12961        1.27443
O          0.35516        1.64406        1.27443
C         -0.12486        2.69408        0.62367
C          2.39557       -1.23891        0.62367
C          0.04588        4.03782        1.02818
C         -0.52942        5.03601        0.21914
N         -1.21099        4.79908       -0.89097
C         -1.38402        3.55477       -1.29742
C         -0.85523        2.49731       -0.56645
C          2.59035       -0.50800       -0.56645
C          3.77053       -0.57879       -1.29742
N          4.76162       -1.35079       -0.89097
C          4.62602       -2.05952        0.21914
C          3.47392       -2.05865        1.02818
F         -2.07274        3.33401       -2.41707
F         -0.98990        1.15518       -0.92485
F         -0.38356        6.30868        0.58772
F          0.72378        4.33531        2.13652
F          3.39260       -2.79446        2.13652
F          5.65526       -2.82217        0.58772
F          3.92370        0.12804       -2.41707
F          1.49537        0.27968       -0.92485

SCF energy GEOOPT =  -2400.707788552 H
ZPE =   393.2 kJ/mol
FREEH energy =   470.46 kJ/mol
FREEH entropy =   0.81449 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
```

#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e	14.05	0.29786	YES	YES
8	e	14.05	0.29786	YES	YES
9	a	26.47	0.69904	YES	YES
10	e	35.68	0.07087	YES	YES
11	e	35.68	0.07087	YES	YES
12	a	41.45	0.00084	YES	YES
13	e	91.98	11.34382	YES	YES
14	e	91.98	11.34382	YES	YES
15	a	93.87	0.00276	YES	YES
16	e	101.96	1.84359	YES	YES
17	e	101.96	1.84359	YES	YES
18	a	124.84	0.92211	YES	YES
19	a	140.67	1.45279	YES	YES
20	e	142.45	0.74224	YES	YES
21	e	142.45	0.74224	YES	YES
22	e	186.90	0.77702	YES	YES
23	e	186.90	0.77702	YES	YES
24	a	195.12	3.26739	YES	YES
25	a	205.33	1.21871	YES	YES
26	a	230.24	20.93808	YES	YES
27	e	230.32	2.03403	YES	YES
28	e	230.32	2.03403	YES	YES
29	e	265.96	36.76070	YES	YES
30	e	265.96	36.76070	YES	YES
31	a	286.97	0.62734	YES	YES
32	e	299.60	3.61881	YES	YES
33	e	299.60	3.61881	YES	YES
34	a	308.60	1.06261	YES	YES
35	e	322.56	12.67745	YES	YES
36	e	322.56	12.67745	YES	YES
37	a	331.58	2.12300	YES	YES
38	e	340.59	29.49849	YES	YES
39	e	340.59	29.49849	YES	YES
40	a	372.43	0.66383	YES	YES
41	e	400.71	12.71517	YES	YES
42	e	400.71	12.71517	YES	YES
43	e	420.76	0.27017	YES	YES
44	e	420.76	0.27017	YES	YES
45	a	421.67	0.33339	YES	YES
46	e	439.53	1.96139	YES	YES
47	e	439.53	1.96139	YES	YES
48	a	439.72	2.56683	YES	YES
49	e	471.63	10.63086	YES	YES
50	e	471.63	10.63086	YES	YES
51	a	475.04	1.28559	YES	YES
52	a	552.38	5.60203	YES	YES
53	e	579.12	24.41914	YES	YES
54	e	579.12	24.41914	YES	YES
55	a	615.69	1.18994	YES	YES
56	e	616.05	1.24705	YES	YES
57	e	616.05	1.24705	YES	YES
58	a	625.64	2.30402	YES	YES
59	e	627.25	3.94609	YES	YES
60	e	627.25	3.94609	YES	YES
61	a	643.78	2.40437	YES	YES
62	e	644.00	3.18568	YES	YES
63	e	644.00	3.18568	YES	YES
64	a	652.62	2.37416	YES	YES
65	e	658.55	2.38822	YES	YES
66	e	658.55	2.38822	YES	YES
67	a	683.74	2.66190	YES	YES
68	e	718.87	87.19088	YES	YES
69	e	718.87	87.19088	YES	YES

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    70        a             741.25          0.00366       YES     YES
    71        e             779.62        176.24608       YES     YES
    72        e             779.62        176.24608       YES     YES
    73        e             951.53        298.95617       YES     YES
    74        e             951.53        298.95617       YES     YES
    75        a             963.64        188.14602       YES     YES
    76        e            1112.23        462.36089       YES     YES
    77        e            1112.23        462.36089       YES     YES
    78        e            1126.45        100.06496       YES     YES
    79        e            1126.45        100.06496       YES     YES
    80        a            1129.33        192.41218       YES     YES
    81        a            1132.17          6.27505       YES     YES
    82        e            1270.11          1.47906       YES     YES
    83        e            1270.11          1.47906       YES     YES
    84        a            1277.27          8.88210       YES     YES
    85        e            1390.02         13.81990       YES     YES
    86        e            1390.02         13.81990       YES     YES
    87        a            1390.28         49.62011       YES     YES
    88        e            1428.07        170.03347       YES     YES
    89        e            1428.07        170.03347       YES     YES
    90        a            1430.59          0.34868       YES     YES
    91        e            1489.83        620.72870       YES     YES
    92        e            1489.83        620.72870       YES     YES
    93        a            1498.07        405.65456       YES     YES
    94        e            1530.94        138.85674       YES     YES
    95        e            1530.94        138.85674       YES     YES
    96        a            1539.84        337.89545       YES     YES
    97        e            1620.46        242.71458       YES     YES
    98        e            1620.46        242.71458       YES     YES
    99        a            1623.06          1.27836       YES     YES
   100        e            1638.13        150.03410       YES     YES
   101        e            1638.13        150.03410       YES     YES
   102        a            1645.66        193.08786       YES     YES
$end
```

$[FAl(OC_5F_4N)_3]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c3

Cartesian coordinates in Ångström:
Al         0.00000        0.00000        2.32338
O         -1.63627       -0.04745        1.60165
C         -2.06597       -0.87052        0.66647
C         -2.20402       -2.26713        0.88228
C         -2.66713       -3.07731       -0.15884
N         -2.99706       -2.61904       -1.35485
C         -2.86817       -1.32341       -1.58427
C         -2.41311       -0.40654       -0.62965
F         -1.87407       -2.78320        2.07763
F         -2.28487        0.89897       -0.92535
F         -3.19848       -0.87658       -2.80917
F         -2.79453       -4.40045        0.05023
O          0.85923       -1.39332        1.60165
O          0.77704        1.44077        1.60165
C          0.27909        2.22445        0.66647
C          1.78688       -1.35393        0.66647
C         -0.86138        3.04230        0.88228
C         -1.33147        3.84846       -0.15884
N         -0.76962        3.90505       -1.35485
C          0.28797        3.14561       -1.58427
C          0.85448        2.29309       -0.62965
C          1.55863       -1.88655       -0.62965
C          2.58019       -1.82220       -1.58427
N          3.76669       -1.28601       -1.35485
C          3.99859       -0.77114       -0.15884
C          3.06540       -0.77517        0.88228
F          0.84011        3.20826       -2.80917
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F          1.92097        1.52927       -0.92535
F         -2.41363        4.62036        0.05023
F         -1.47329        3.01459        2.07763
F          3.34736       -0.23139        2.07763
F          5.20817       -0.21991        0.05023
F          2.35838       -2.33168       -2.80917
F          0.36390       -2.42824       -0.92535
F          0.00000       -0.00000        4.00186

SCF energy GEOOPT =  -2500.686346194 H
ZPE =   398.8 kJ/mol
FREEH energy =   480.82 kJ/mol
FREEH entropy =   0.85687 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        e             18.06         0.00539       YES     YES
     8        e             18.06         0.00539       YES     YES
     9        a             24.92         0.05302       YES     YES
    10        e             34.12         0.01000       YES     YES
    11        e             34.12         0.01000       YES     YES
    12        a             34.66         0.01078       YES     YES
    13        e             44.91         0.04360       YES     YES
    14        e             44.91         0.04360       YES     YES
    15        a             47.65         0.12485       YES     YES
    16        e             94.63         0.98659       YES     YES
    17        e             94.63         0.98659       YES     YES
    18        a            107.12         0.18039       YES     YES
    19        a            118.91         0.09593       YES     YES
    20        e            119.84         0.05125       YES     YES
    21        e            119.84         0.05125       YES     YES
    22        e            148.84         0.38604       YES     YES
    23        e            148.84         0.38604       YES     YES
    24        e            193.44        10.02055       YES     YES
    25        e            193.44        10.02055       YES     YES
    26        a            202.65         0.75427       YES     YES
    27        e            221.49         0.30843       YES     YES
    28        e            221.49         0.30843       YES     YES
    29        a            241.41         8.78764       YES     YES
    30        e            270.38         3.98134       YES     YES
    31        e            270.38         3.98134       YES     YES
    32        a            273.39         1.55726       YES     YES
    33        a            289.20         6.12469       YES     YES
    34        e            292.07         1.62393       YES     YES
    35        e            292.07         1.62393       YES     YES
    36        a            315.19         7.03882       YES     YES
    37        e            330.00        13.80410       YES     YES
    38        e            330.00        13.80410       YES     YES
    39        a            339.06         4.24120       YES     YES
    40        e            343.08         2.32425       YES     YES
    41        e            343.08         2.32425       YES     YES
    42        a            352.33         6.54857       YES     YES
    43        e            360.73         6.02004       YES     YES
    44        e            360.73         6.02004       YES     YES
    45        a            425.25         0.46962       YES     YES
    46        e            432.86         0.51593       YES     YES
    47        e            432.86         0.51593       YES     YES
    48        a            433.26         0.00011       YES     YES
    49        e            447.17         5.16317       YES     YES
    50        e            447.17         5.16317       YES     YES
    51        a            448.69         0.00157       YES     YES
    52        e            460.17        22.72292       YES     YES
    53        e            460.17        22.72292       YES     YES
```

54	a	513.55	0.00823	YES	YES
55	e	547.05	56.28734	YES	YES
56	e	547.05	56.28734	YES	YES
57	a	623.43	0.00451	YES	YES
58	e	624.30	3.89540	YES	YES
59	e	624.30	3.89540	YES	YES
60	e	632.69	0.48718	YES	YES
61	e	632.69	0.48718	YES	YES
62	a	632.86	0.02881	YES	YES
63	a	644.38	0.90267	YES	YES
64	e	646.56	3.27577	YES	YES
65	e	646.56	3.27577	YES	YES
66	a	664.49	7.46684	YES	YES
67	e	674.77	7.44794	YES	YES
68	e	674.77	7.44794	YES	YES
69	a	693.71	1.19314	YES	YES
70	e	725.15	13.10311	YES	YES
71	e	725.15	13.10311	YES	YES
72	a	729.30	0.97170	YES	YES
73	e	746.22	91.19274	YES	YES
74	e	746.22	91.19274	YES	YES
75	a	873.30	155.01362	YES	YES
76	a	967.73	184.00017	YES	YES
77	e	968.67	179.26552	YES	YES
78	e	968.67	179.26552	YES	YES
79	e	1119.96	355.10220	YES	YES
80	e	1119.96	355.10220	YES	YES
81	a	1133.03	361.17006	YES	YES
82	e	1148.17	0.52952	YES	YES
83	e	1148.17	0.52952	YES	YES
84	a	1148.90	3.33830	YES	YES
85	e	1299.91	2.02281	YES	YES
86	e	1299.91	2.02281	YES	YES
87	a	1303.60	16.45926	YES	YES
88	e	1375.63	18.07524	YES	YES
89	e	1375.63	18.07524	YES	YES
90	a	1376.07	26.30256	YES	YES
91	e	1419.59	30.46054	YES	YES
92	e	1419.59	30.46054	YES	YES
93	a	1421.80	37.68010	YES	YES
94	a	1487.07	499.50956	YES	YES
95	e	1487.96	424.70578	YES	YES
96	e	1487.96	424.70578	YES	YES
97	e	1541.42	404.92452	YES	YES
98	e	1541.42	404.92452	YES	YES
99	a	1560.23	331.59440	YES	YES
100	e	1605.70	5.49426	YES	YES
101	e	1605.70	5.49426	YES	YES
102	a	1606.09	3.58819	YES	YES
103	e	1625.87	163.11157	YES	YES
104	e	1625.87	163.11157	YES	YES
105	a	1635.75	252.67492	YES	YES

$end

$Al(OC_{10}F_{15})_3$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

C	-2.91631	-2.83123	-2.23530
C	-2.27445	-4.21625	-1.90720
C	-0.81407	-4.27060	-2.46437
C	-0.82074	-4.04412	-4.01002
C	-1.44256	-2.64633	-4.33345
C	-2.91160	-2.61248	-3.79428
C	-0.59060	-1.51086	-3.65444
C	0.02182	-3.14138	-1.79744

C	-2.07397	-1.68854	-1.62532
C	-0.58573	-1.71489	-2.10007
F	-2.27644	-4.40244	-0.56517
F	-3.01589	-5.20977	-2.44461
F	-0.26836	-5.48845	-2.18515
F	-1.52607	-5.02463	-4.62076
F	0.44100	-4.11542	-4.49234
F	-1.45673	-2.45685	-5.68271
F	-3.49598	-1.43309	-4.10222
F	-3.65107	-3.57814	-4.38449
F	-4.19524	-2.79076	-1.77042
F	-1.11543	-0.30464	-3.97000
F	0.67034	-1.53222	-4.13873
F	0.05225	-3.33928	-0.45421
F	1.30299	-3.18799	-2.22132
F	-2.65680	-0.50481	-1.88545
F	-2.01867	-1.73480	-0.22121
O	0.11675	-0.74706	-1.43656
Al	-0.20824	-0.30755	0.23187
C	2.53112	-0.08730	4.15362
C	3.57627	0.43626	3.11332
C	3.75565	-0.60596	1.96264
C	4.22018	-1.98219	2.57064
C	3.14977	-2.50228	3.58811
C	3.00281	-1.45648	4.74138
C	1.76414	-2.70513	2.86500
C	2.40798	-0.87802	1.27113
C	1.16876	-0.29780	3.43736
C	1.28853	-1.33927	2.25609
F	3.16641	1.61478	2.58752
F	4.76355	0.66170	3.71589
F	4.68015	-0.15729	1.07074
F	5.41492	-1.81894	3.17974
F	4.40585	-2.89091	1.58813
F	3.56873	-3.69161	4.10283
F	2.11443	-1.90102	5.65801
F	4.18404	-1.30137	5.38456
F	2.40053	0.82406	5.15791
F	0.85640	-3.18099	3.74279
F	1.89916	-3.63593	1.89215
F	1.87525	0.27728	0.63675
F	2.56689	-1.74429	0.25777
F	0.23366	-0.71814	4.31503
F	0.72883	0.88559	2.93792
O	0.10630	-1.40932	1.57332
O	-1.03140	1.16385	0.56454
F	-1.30183	1.95896	-2.13882
F	-3.15329	2.10276	-1.00992
F	1.03887	3.00763	1.12245
F	0.97793	2.41921	-0.96496
F	-1.18752	3.17170	2.48962
F	-3.08918	2.76427	1.52168
F	-2.74829	4.25561	-2.70960
F	-4.03172	4.43122	-0.25026
F	-2.91765	6.22689	-0.74953
F	-2.62201	5.47590	1.91179
F	0.15755	5.32474	1.87356
F	-0.63377	6.70943	0.40241
F	1.44173	5.14320	-0.58522
F	0.03253	4.09608	-2.74167
F	-0.69633	6.04367	-2.11868
C	-1.11440	2.47313	0.19635
C	-1.92024	2.64393	-1.14444
C	0.30293	3.11830	-0.00865
C	-1.85641	3.28437	1.31774
C	-2.78136	4.92279	-0.41081
C	-1.97682	4.79386	0.92358
C	-0.54804	5.39665	0.72143
C	0.19455	4.61902	-0.41431
C	-0.61308	4.74558	-1.74555

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C         -2.04326        4.14638       -1.54767

SCF energy GEOOPT =  -6100.247518346 H
ZPE =   867.7 kJ/mol
FREEH energy =  1042.73 kJ/mol
FREEH entropy =   1.42939 kJ/mol/K

$vibrational spectrum
```

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.76	0.23397	YES	YES
8	a	18.88	0.07842	YES	YES
9	a	19.08	0.14625	YES	YES
10	a	24.13	0.08407	YES	YES
11	a	25.39	0.01673	YES	YES
12	a	26.41	0.68887	YES	YES
13	a	38.06	4.65712	YES	YES
14	a	49.01	0.84367	YES	YES
15	a	54.29	1.12609	YES	YES
16	a	64.60	2.59757	YES	YES
17	a	67.99	1.99159	YES	YES
18	a	88.70	0.03155	YES	YES
19	a	126.61	27.93387	YES	YES
20	a	127.34	8.02082	YES	YES
21	a	132.76	3.56686	YES	YES
22	a	135.13	0.08774	YES	YES
23	a	135.22	0.38547	YES	YES
24	a	137.01	1.97931	YES	YES
25	a	139.90	0.36623	YES	YES
26	a	141.64	9.70222	YES	YES
27	a	145.39	12.94775	YES	YES
28	a	153.87	45.58389	YES	YES
29	a	188.97	1.80045	YES	YES
30	a	191.24	0.37717	YES	YES
31	a	193.37	2.37474	YES	YES
32	a	194.46	1.40470	YES	YES
33	a	197.03	1.20132	YES	YES
34	a	198.01	0.37729	YES	YES
35	a	199.73	1.64790	YES	YES
36	a	199.98	1.59497	YES	YES
37	a	200.83	0.62489	YES	YES
38	a	202.28	2.00929	YES	YES
39	a	203.18	0.31777	YES	YES
40	a	205.11	0.21857	YES	YES
41	a	206.25	0.99976	YES	YES
42	a	209.21	0.78063	YES	YES
43	a	210.44	0.21986	YES	YES
44	a	224.29	0.04171	YES	YES
45	a	224.50	0.08751	YES	YES
46	a	226.23	0.25160	YES	YES
47	a	237.49	3.44721	YES	YES
48	a	241.08	1.55689	YES	YES
49	a	241.19	0.07381	YES	YES
50	a	241.80	0.88088	YES	YES
51	a	242.68	0.63126	YES	YES
52	a	243.73	1.08242	YES	YES
53	a	244.40	0.19052	YES	YES
54	a	244.62	0.05675	YES	YES
55	a	244.84	1.15408	YES	YES
56	a	245.34	0.33353	YES	YES
57	a	245.51	0.37192	YES	YES
58	a	245.73	0.54104	YES	YES
59	a	246.48	0.10036	YES	YES
60	a	246.98	0.28320	YES	YES

61	a	250.03	4.47063	YES	YES
62	a	250.26	0.77336	YES	YES
63	a	251.19	2.28939	YES	YES
64	a	253.54	2.67821	YES	YES
65	a	254.49	0.89243	YES	YES
66	a	255.40	1.56636	YES	YES
67	a	256.24	0.70034	YES	YES
68	a	256.99	0.90549	YES	YES
69	a	257.55	1.18649	YES	YES
70	a	257.92	1.14940	YES	YES
71	a	261.74	0.38535	YES	YES
72	a	262.41	0.06522	YES	YES
73	a	263.87	1.41719	YES	YES
74	a	276.07	17.29598	YES	YES
75	a	278.32	14.20623	YES	YES
76	a	284.69	9.72549	YES	YES
77	a	292.91	9.43059	YES	YES
78	a	293.24	5.11274	YES	YES
79	a	294.56	3.48180	YES	YES
80	a	295.48	1.41023	YES	YES
81	a	295.65	3.20000	YES	YES
82	a	296.51	3.39840	YES	YES
83	a	297.10	0.71909	YES	YES
84	a	297.96	12.33843	YES	YES
85	a	299.63	1.34134	YES	YES
86	a	300.17	9.98249	YES	YES
87	a	300.28	13.15031	YES	YES
88	a	303.77	1.22987	YES	YES
89	a	307.55	0.39162	YES	YES
90	a	313.84	11.14796	YES	YES
91	a	316.96	0.67144	YES	YES
92	a	336.01	5.00973	YES	YES
93	a	349.98	27.18399	YES	YES
94	a	362.19	0.45762	YES	YES
95	a	364.12	0.11059	YES	YES
96	a	364.76	4.79936	YES	YES
97	a	371.55	10.25039	YES	YES
98	a	376.47	2.89950	YES	YES
99	a	377.20	0.52124	YES	YES
100	a	377.37	2.28157	YES	YES
101	a	377.46	0.21168	YES	YES
102	a	378.40	1.18708	YES	YES
103	a	378.60	1.34755	YES	YES
104	a	378.91	0.34916	YES	YES
105	a	381.50	1.11892	YES	YES
106	a	382.13	1.18247	YES	YES
107	a	384.62	3.93514	YES	YES
108	a	384.80	6.55920	YES	YES
109	a	387.52	1.02373	YES	YES
110	a	388.36	7.05288	YES	YES
111	a	390.77	18.18965	YES	YES
112	a	391.87	16.08437	YES	YES
113	a	411.77	0.00068	YES	YES
114	a	418.90	5.53407	YES	YES
115	a	428.17	0.19185	YES	YES
116	a	429.80	11.60605	YES	YES
117	a	430.56	15.08423	YES	YES
118	a	432.42	13.41973	YES	YES
119	a	432.55	2.77540	YES	YES
120	a	433.80	8.87811	YES	YES
121	a	435.95	23.30833	YES	YES
122	a	439.05	5.83166	YES	YES
123	a	445.05	3.91756	YES	YES
124	a	512.06	2.39272	YES	YES
125	a	542.85	6.60524	YES	YES
126	a	552.20	3.88531	YES	YES
127	a	586.12	2.14502	YES	YES
128	a	588.21	1.19891	YES	YES
129	a	589.11	0.12250	YES	YES
130	a	589.73	0.14163	YES	YES

131	a	590.14	0.17717	YES	YES
132	a	591.27	0.24308	YES	YES
133	a	616.31	6.22457	YES	YES
134	a	628.29	13.07545	YES	YES
135	a	630.31	20.28725	YES	YES
136	a	633.57	5.01758	YES	YES
137	a	635.07	28.47172	YES	YES
138	a	635.52	4.14421	YES	YES
139	a	636.20	13.91054	YES	YES
140	a	636.24	14.92744	YES	YES
141	a	636.83	15.68519	YES	YES
142	a	648.91	0.45856	YES	YES
143	a	674.31	13.49422	YES	YES
144	a	677.06	17.63262	YES	YES
145	a	701.15	1.15167	YES	YES
146	a	790.52	53.50633	YES	YES
147	a	809.68	18.27694	YES	YES
148	a	829.74	6.71186	YES	YES
149	a	831.37	2.18275	YES	YES
150	a	834.26	0.06982	YES	YES
151	a	834.97	0.00863	YES	YES
152	a	836.23	0.27433	YES	YES
153	a	836.59	0.49521	YES	YES
154	a	837.78	0.29101	YES	YES
155	a	843.79	1.82511	YES	YES
156	a	847.45	2.05541	YES	YES
157	a	912.77	216.39422	YES	YES
158	a	932.72	239.81449	YES	YES
159	a	956.99	22.70828	YES	YES
160	a	959.48	51.62407	YES	YES
161	a	961.90	377.51175	YES	YES
162	a	963.24	522.93314	YES	YES
163	a	968.01	451.99588	YES	YES
164	a	968.71	200.93718	YES	YES
165	a	976.85	232.93692	YES	YES
166	a	978.06	248.05291	YES	YES
167	a	979.47	178.32349	YES	YES
168	a	985.47	8.28479	YES	YES
169	a	988.55	8.99672	YES	YES
170	a	989.21	15.18248	YES	YES
171	a	989.49	2.09472	YES	YES
172	a	1021.02	28.32402	YES	YES
173	a	1024.28	35.45597	YES	YES
174	a	1040.02	9.67138	YES	YES
175	a	1040.77	2.25396	YES	YES
176	a	1042.34	3.59681	YES	YES
177	a	1045.60	4.11170	YES	YES
178	a	1048.01	8.67520	YES	YES
179	a	1048.29	23.24253	YES	YES
180	a	1052.37	2.66676	YES	YES
181	a	1053.13	2.19982	YES	YES
182	a	1053.36	0.44911	YES	YES
183	a	1055.87	0.53689	YES	YES
184	a	1058.54	1.72857	YES	YES
185	a	1063.58	19.22691	YES	YES
186	a	1064.69	12.67592	YES	YES
187	a	1080.95	12.93561	YES	YES
188	a	1087.40	2.10834	YES	YES
189	a	1095.47	64.69433	YES	YES
190	a	1098.87	66.65373	YES	YES
191	a	1105.15	51.26535	YES	YES
192	a	1121.63	2.60210	YES	YES
193	a	1129.02	0.41857	YES	YES
194	a	1130.11	5.09455	YES	YES
195	a	1130.45	2.27272	YES	YES
196	a	1132.17	0.44815	YES	YES
197	a	1137.12	1.20697	YES	YES
198	a	1139.95	1.43473	YES	YES
199	a	1189.48	9.83738	YES	YES
200	a	1191.02	42.14299	YES	YES

201	a	1199.57	6.49742	YES	YES
202	a	1205.04	7.86489	YES	YES
203	a	1206.04	0.89019	YES	YES
204	a	1206.61	7.00041	YES	YES
205	a	1207.40	6.68185	YES	YES
206	a	1208.62	5.24116	YES	YES
207	a	1209.63	17.84937	YES	YES
208	a	1210.09	1.86689	YES	YES
209	a	1210.44	19.55814	YES	YES
210	a	1211.93	27.85729	YES	YES
211	a	1212.28	21.34574	YES	YES
212	a	1214.51	50.78448	YES	YES
213	a	1216.20	51.37073	YES	YES
214	a	1230.53	80.98411	YES	YES
215	a	1232.94	271.92885	YES	YES
216	a	1237.89	20.57881	YES	YES
217	a	1249.05	430.83241	YES	YES
218	a	1249.58	204.21067	YES	YES
219	a	1252.23	348.17249	YES	YES
220	a	1257.32	380.68263	YES	YES
221	a	1260.62	220.33564	YES	YES
222	a	1260.87	266.08602	YES	YES
223	a	1261.08	12.96067	YES	YES
224	a	1261.29	286.43836	YES	YES
225	a	1262.53	40.29781	YES	YES
226	a	1263.14	158.41274	YES	YES
227	a	1264.91	62.69831	YES	YES
228	a	1266.15	59.32786	YES	YES
229	a	1266.44	603.65721	YES	YES
230	a	1269.71	402.22886	YES	YES
231	a	1270.92	196.40491	YES	YES
232	a	1277.11	56.32074	YES	YES
233	a	1280.08	193.46838	YES	YES
234	a	1287.25	43.02739	YES	YES
235	a	1315.09	44.83788	YES	YES
236	a	1315.61	45.64344	YES	YES
237	a	1344.78	227.76617	YES	YES

$end

$[FAl(OC_{10}F_{15})_3]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

C	-5.20503	-2.73775	0.90851
C	-4.95176	-1.27057	0.44488
C	-3.98749	-3.63012	0.51854
F	-6.34298	-3.22141	0.34247
F	-5.40871	-2.77837	2.24776
C	-4.76100	-1.24302	-1.10308
C	-3.80004	-3.59748	-1.02895
C	-3.54125	-2.13166	-1.49632
F	-4.57642	0.02618	-1.53415
F	-5.88733	-1.69227	-1.72072
F	-4.90369	-4.10108	-1.64456
F	-2.76951	-4.39624	-1.39450
C	-3.66089	-0.72229	1.13410
F	-6.03424	-0.50236	0.77972
C	-2.69902	-3.07898	1.20908
F	-4.22746	-4.91877	0.91582
C	-2.25075	-1.58781	-0.79980
F	-3.38962	-2.11337	-2.85628
C	-2.39174	-1.59302	0.77301
F	-3.84309	-0.70880	2.47853
F	-3.47258	0.56479	0.75787
F	-1.65048	-3.87997	0.90022
F	-2.85294	-3.14733	2.55462

```
F         -2.00332       -0.32914       -1.24141
F         -1.19261       -2.34340       -1.17713
O         -1.29834       -1.16547        1.41586
F          1.41620        2.06355       -1.14223
F          2.82995        4.14487       -0.52449
F          1.83643        2.66209        1.37419
F          1.19417        4.29498       -2.77461
C          0.29607        2.82009       -1.09364
F         -0.56963        2.29423       -1.99471
O         -0.69317        1.52524        0.70361
C          1.68758        4.86863       -0.50625
C          0.65443        4.28101       -1.51648
C          0.70694        3.41528        1.34545
C         -0.33679        2.76778        0.35508
F          2.03448        6.13246       -0.87164
F          1.98133        5.40526        1.80474
C          1.07387        4.87450        0.92838
F          0.21521        3.42651        2.60714
C         -0.63522        5.15561       -1.50336
F         -1.53199        4.68320       -2.40155
C         -1.61143        3.69624        0.34540
F         -2.54006        3.20625       -0.51116
F         -0.34640        6.42678       -1.89284
C         -0.21775        5.74910        0.93384
C         -1.25406        5.15984       -0.07158
F         -2.18724        3.71268        1.57329
F          0.08367        7.03282        0.59985
F         -0.74751        5.80268        2.17922
F         -2.37803        5.94126       -0.06998
F          3.74404        0.67384        0.18674
F          5.39716       -0.37404       -1.52432
F          2.85891       -0.26463       -2.09569
F          5.90399       -0.76675        1.18391
C          3.54957       -0.55505        0.72614
F          3.30357       -0.36471        2.04355
O          1.19728       -0.52230        0.12836
C          5.17705       -1.57776       -0.94327
C          4.85523       -1.39771        0.57143
C          2.68692       -1.46232       -1.48561
C          2.31478       -1.25518        0.03343
F          6.32842       -2.28587       -1.09832
F          4.28890       -2.47345       -2.97357
C          3.99380       -2.30862       -1.64661
F          1.67385       -2.08447       -2.13523
C          4.64515       -2.79770        1.22820
F          4.39517       -2.66447        2.55198
C          2.15893       -2.68966        0.67460
F          1.84327       -2.57271        1.99007
F          5.78332       -3.53637        1.13233
C          3.79249       -3.70845       -0.98896
C          3.46400       -3.53452        0.52686
F          1.13426       -3.35364        0.09035
F          4.91227       -4.46591       -1.14062
F          2.79790       -4.38043       -1.61466
F          3.30052       -4.76869        1.09571
Al         0.01256        0.02501        1.33458
F          0.62787        0.22333        2.88887

SCF energy GEOOPT =  -6200.226682947 H
ZPE =   871.3 kJ/mol
FREEH energy =  1051.05 kJ/mol
FREEH entropy =   1.47869 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
```

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.29	0.12334	YES	YES
8	a	12.89	0.00039	YES	YES
9	a	15.59	0.04729	YES	YES
10	a	17.41	0.04949	YES	YES
11	a	19.74	0.06387	YES	YES
12	a	20.60	0.00543	YES	YES
13	a	35.66	0.01309	YES	YES
14	a	41.63	0.00796	YES	YES
15	a	43.34	0.01620	YES	YES
16	a	56.17	0.15084	YES	YES
17	a	60.48	0.37713	YES	YES
18	a	72.99	0.41039	YES	YES
19	a	121.70	1.98830	YES	YES
20	a	122.77	1.48294	YES	YES
21	a	131.50	0.00434	YES	YES
22	a	132.95	0.02768	YES	YES
23	a	133.09	0.00261	YES	YES
24	a	134.16	0.00087	YES	YES
25	a	136.97	0.05934	YES	YES
26	a	139.56	0.09533	YES	YES
27	a	141.81	0.59308	YES	YES
28	a	148.83	2.84336	YES	YES
29	a	149.70	3.85764	YES	YES
30	a	184.28	1.19188	YES	YES
31	a	193.90	0.50425	YES	YES
32	a	194.61	0.48980	YES	YES
33	a	195.54	0.31580	YES	YES
34	a	196.36	0.34268	YES	YES
35	a	196.90	0.57314	YES	YES
36	a	197.82	0.50215	YES	YES
37	a	198.46	0.40662	YES	YES
38	a	199.72	0.91988	YES	YES
39	a	201.13	0.06020	YES	YES
40	a	201.92	0.03915	YES	YES
41	a	202.57	0.11322	YES	YES
42	a	203.15	0.07829	YES	YES
43	a	203.28	0.06884	YES	YES
44	a	204.79	0.12893	YES	YES
45	a	212.48	0.59143	YES	YES
46	a	224.12	0.01084	YES	YES
47	a	224.73	0.00454	YES	YES
48	a	225.56	0.01488	YES	YES
49	a	242.19	0.22205	YES	YES
50	a	243.17	0.09045	YES	YES
51	a	243.57	0.86511	YES	YES
52	a	243.97	0.36105	YES	YES
53	a	244.22	0.29188	YES	YES
54	a	244.45	0.09905	YES	YES
55	a	244.71	0.07805	YES	YES
56	a	244.89	0.02523	YES	YES
57	a	244.94	0.04376	YES	YES
58	a	245.28	0.22020	YES	YES
59	a	245.70	0.80298	YES	YES
60	a	246.06	0.08773	YES	YES
61	a	246.15	0.18717	YES	YES
62	a	246.84	0.46956	YES	YES
63	a	247.45	0.03026	YES	YES
64	a	250.33	3.17264	YES	YES
65	a	251.63	3.71315	YES	YES
66	a	251.73	0.86364	YES	YES
67	a	255.19	0.59464	YES	YES
68	a	256.60	0.28910	YES	YES
69	a	257.24	0.54406	YES	YES
70	a	258.02	0.09824	YES	YES
71	a	258.15	0.96533	YES	YES
72	a	259.72	0.52799	YES	YES
73	a	263.32	0.00106	YES	YES
74	a	263.76	0.09855	YES	YES

75	a	264.26	0.09890	YES	YES
76	a	267.60	0.97129	YES	YES
77	a	278.34	13.36716	YES	YES
78	a	283.98	12.81722	YES	YES
79	a	290.05	8.06378	YES	YES
80	a	293.38	9.32776	YES	YES
81	a	294.81	9.25083	YES	YES
82	a	295.79	8.32911	YES	YES
83	a	296.31	9.19526	YES	YES
84	a	296.54	0.56620	YES	YES
85	a	297.01	8.03511	YES	YES
86	a	297.26	5.80538	YES	YES
87	a	297.36	4.84259	YES	YES
88	a	297.52	4.64406	YES	YES
89	a	298.15	5.62260	YES	YES
90	a	299.73	0.68893	YES	YES
91	a	301.05	0.70337	YES	YES
92	a	308.35	0.42352	YES	YES
93	a	311.22	1.68040	YES	YES
94	a	317.94	10.77880	YES	YES
95	a	338.93	38.50438	YES	YES
96	a	359.55	11.20004	YES	YES
97	a	361.57	0.16626	YES	YES
98	a	362.30	0.42559	YES	YES
99	a	364.21	12.23733	YES	YES
100	a	374.64	0.27669	YES	YES
101	a	374.92	0.02052	YES	YES
102	a	375.57	0.30771	YES	YES
103	a	376.14	0.58527	YES	YES
104	a	376.73	3.38746	YES	YES
105	a	376.80	2.52275	YES	YES
106	a	376.89	0.32750	YES	YES
107	a	377.27	3.66125	YES	YES
108	a	377.65	0.69397	YES	YES
109	a	379.40	10.31943	YES	YES
110	a	380.60	10.55828	YES	YES
111	a	385.93	2.30965	YES	YES
112	a	387.25	1.03391	YES	YES
113	a	387.98	14.02567	YES	YES
114	a	388.83	13.31554	YES	YES
115	a	395.87	29.73662	YES	YES
116	a	397.11	22.29706	YES	YES
117	a	428.57	0.19322	YES	YES
118	a	429.70	11.05833	YES	YES
119	a	429.85	8.87330	YES	YES
120	a	430.79	8.90372	YES	YES
121	a	431.38	4.45722	YES	YES
122	a	432.01	10.53376	YES	YES
123	a	433.23	15.64991	YES	YES
124	a	434.65	25.72008	YES	YES
125	a	435.18	23.18005	YES	YES
126	a	497.96	3.38074	YES	YES
127	a	524.84	23.36316	YES	YES
128	a	525.51	25.87477	YES	YES
129	a	588.25	0.07044	YES	YES
130	a	588.42	0.03128	YES	YES
131	a	588.96	0.02870	YES	YES
132	a	589.23	0.05485	YES	YES
133	a	589.46	0.02760	YES	YES
134	a	589.76	0.28254	YES	YES
135	a	611.77	4.10515	YES	YES
136	a	627.76	10.02658	YES	YES
137	a	627.97	9.99758	YES	YES
138	a	633.86	1.11438	YES	YES
139	a	634.29	14.68197	YES	YES
140	a	634.40	18.14296	YES	YES
141	a	634.76	4.05898	YES	YES
142	a	634.94	6.05495	YES	YES
143	a	635.36	28.38732	YES	YES
144	a	647.56	0.43922	YES	YES

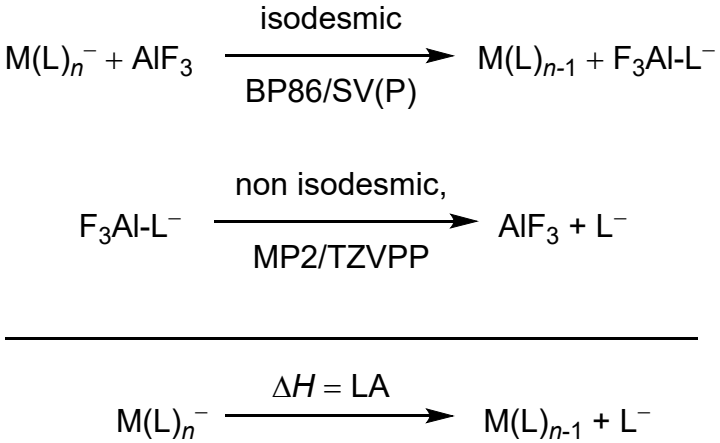
145	a	664.37	26.93513	YES	YES
146	a	664.87	28.16264	YES	YES
147	a	702.28	2.19593	YES	YES
148	a	743.14	39.97518	YES	YES
149	a	745.83	42.54068	YES	YES
150	a	831.41	3.75813	YES	YES
151	a	832.25	1.46476	YES	YES
152	a	832.91	1.59597	YES	YES
153	a	834.22	0.02396	YES	YES
154	a	835.03	3.56075	YES	YES
155	a	835.46	0.02529	YES	YES
156	a	835.55	0.01764	YES	YES
157	a	835.91	0.52201	YES	YES
158	a	837.13	0.54049	YES	YES
159	a	844.82	53.37707	YES	YES
160	a	952.23	49.08501	YES	YES
161	a	954.68	39.22396	YES	YES
162	a	955.50	81.81492	YES	YES
163	a	958.53	447.41900	YES	YES
164	a	959.80	563.91484	YES	YES
165	a	960.97	457.58318	YES	YES
166	a	969.07	499.26657	YES	YES
167	a	969.21	539.28635	YES	YES
168	a	975.25	72.77593	YES	YES
169	a	979.20	19.92077	YES	YES
170	a	979.55	16.77431	YES	YES
171	a	979.94	24.36020	YES	YES
172	a	982.78	7.65133	YES	YES
173	a	983.36	11.89531	YES	YES
174	a	984.32	8.72487	YES	YES
175	a	1020.88	1.49960	YES	YES
176	a	1021.70	1.81030	YES	YES
177	a	1022.85	3.48998	YES	YES
178	a	1025.07	1.28862	YES	YES
179	a	1025.42	3.25000	YES	YES
180	a	1027.52	1.33056	YES	YES
181	a	1053.09	1.09888	YES	YES
182	a	1053.63	1.42145	YES	YES
183	a	1054.04	1.09650	YES	YES
184	a	1054.87	1.19899	YES	YES
185	a	1055.19	1.53456	YES	YES
186	a	1056.23	1.47283	YES	YES
187	a	1066.12	0.37136	YES	YES
188	a	1066.66	0.38126	YES	YES
189	a	1067.18	0.31291	YES	YES
190	a	1088.30	75.97481	YES	YES
191	a	1089.26	75.67297	YES	YES
192	a	1092.91	4.34242	YES	YES
193	a	1116.87	0.23205	YES	YES
194	a	1117.90	0.42132	YES	YES
195	a	1118.18	0.32565	YES	YES
196	a	1118.77	1.03942	YES	YES
197	a	1119.77	0.42824	YES	YES
198	a	1120.62	1.16299	YES	YES
199	a	1127.43	0.26665	YES	YES
200	a	1129.29	0.08178	YES	YES
201	a	1129.85	0.02509	YES	YES
202	a	1195.76	2.98183	YES	YES
203	a	1196.53	0.35146	YES	YES
204	a	1199.18	3.33823	YES	YES
205	a	1200.13	2.27366	YES	YES
206	a	1200.75	0.21018	YES	YES
207	a	1203.23	11.29993	YES	YES
208	a	1204.10	1.55172	YES	YES
209	a	1205.81	10.64430	YES	YES
210	a	1206.09	9.56011	YES	YES
211	a	1206.47	4.98935	YES	YES
212	a	1206.91	27.85608	YES	YES
213	a	1207.85	7.90939	YES	YES
214	a	1209.69	8.40160	YES	YES

215	a	1209.77	0.68183	YES	YES
216	a	1210.02	16.46687	YES	YES
217	a	1231.17	9.62689	YES	YES
218	a	1231.23	11.12999	YES	YES
219	a	1232.53	5.25969	YES	YES
220	a	1245.41	55.85335	YES	YES
221	a	1246.99	902.48038	YES	YES
222	a	1247.23	915.57567	YES	YES
223	a	1249.99	193.70358	YES	YES
224	a	1250.45	92.25906	YES	YES
225	a	1251.01	21.02633	YES	YES
226	a	1252.08	46.60999	YES	YES
227	a	1252.70	4.00033	YES	YES
228	a	1253.40	34.61105	YES	YES
229	a	1253.96	139.88130	YES	YES
230	a	1254.13	87.30021	YES	YES
231	a	1254.93	81.80924	YES	YES
232	a	1257.64	825.41839	YES	YES
233	a	1260.70	285.49650	YES	YES
234	a	1262.07	242.86473	YES	YES
235	a	1278.52	139.33406	YES	YES
236	a	1279.06	158.03210	YES	YES
237	a	1285.88	12.65170	YES	YES
238	a	1355.56	408.30886	YES	YES
239	a	1359.84	447.19245	YES	YES
240	a	1383.42	49.65496	YES	YES

$end

Ligand Affinity (LA)

The LA was calculated in two parts, Scheme S- 2. The first describes an isodesmic reaction on BP86(D3BJ)/def-SV(P) level of theory allowing reliable calculations also for very large systems. The second reaction is non isodesmic containing smaller molecules, hence calculated on the more reliable MP2/def-TZVPP[17] level of theory. Addition of both reaction enthalpies yields the ligand affinity.



Scheme S- 2: Underlying reactions for calculating the ligand affinity LA.

Table S- 6: Summary of thermodynamic data calculated at the BP86(D3BJ)/def-SV(P) level of theory (grid m3, 298.15 K) for the calculation of the isodesmic reaction:

	E_{SCF} / H	E_{SCF} / kJ·mol^{-1}	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	$G°$ / kJ·mol^{-1}	$H°$ / kJ·mol^{-1}
$[Al(C_6F_5)_4]^-$	-3151.86	-8275217.15	613.86	1.05443	-8274915.19	-8274600.81
$[B(C_6F_5)_4]^-$	-2934.29	-7703974.93	624.23	0.97863	-7703640.00	-7703348.22
$[B(OCH(CF_3)_2)_4]^-$	-3179.83	-8348641.63	652.36	1.07771	-8348308.11	-8347986.79
$[Al(OC(CF_3)_3)_4]^-$	-4744.67	-12457137.25	721.13	1.33929	-12456812.95	-12456413.64
$[Al(OC_5F_4N)_4]^-$	-3120.30	-8192333.59	627.22	1.08267	-8192026.69	-8191703.90
$[B(OC_5F_4N)_4]^-$	-2902.67	-7620948.52	634.84	1.01136	-7620612.74	-7620311.20
$[Al(OTeF_5)_4]^-$	-2571.17	-6750602.73	265.95	1.07522	-6750654.88	-6750334.30
$[Ga(OTeF_5)_4]^-$	-4253.59	-11167790.50	263.06	1.06350	-11167842.04	-11167524.96
$[Al(OC_{10}F_{15})_4]^-$	-8053.02	-21143201.57	1389.24	1.84778	-21142360.77	-21141809.85
$[Ga(C_2F_5)_4]^-$	-4225.13	-11093074.62	344.32	0.84508	-11092979.78	-11092727.82
$Al(C_6F_5)_3$	-2424.39	-6365246.54	463.17	0.87140	-6365040.69	-6364780.89
$B(C_6F_5)_3$	-2206.83	-5794041.26	472.69	0.81730	-5793809.77	-5793566.09
$B(OCH(CF_3)_2)_3$	-2391.01	-6277606.11	497.71	0.88587	-6277370.04	-6277105.92
$Al(OC(CF_3)_3)_3$	-3619.01	-9501700.91	541.91	1.05638	-9501471.48	-9501156.52
$Al(OC_5F_4N)_3$	-2400.71	-6303057.10	470.46	0.81449	-6302827.00	-6302584.16
$B(OC_5F_4N)_3$	-2183.11	-5731765.27	482.91	0.84514	-5731531.86	-5731279.88
$Al(OTeF_5)_3$	-1988.88	-5221794.53	199.43	0.79318	-5221829.11	-5221592.62
$Ga(OTeF_5)_3$	-3671.29	-9638964.99	197.06	0.81575	-9639008.66	-9638765.45
$Al(OC_{10}F_{15})_3$	-6100.25	-16016196.81	1042.73	1.42939	-16015577.77	-16015151.60
$Ga(C_2F_5)_3$	-3649.97	-9582982.68	260.03	0.72732	-9582937.02	-9582720.17
AlF_3	-541.89	-1422737.58	31.87	0.29439	-1422791.00	-1422703.23
$F_3Al\text{-}C_6F_5$	-1269.34	-3332648.20	182.96	0.51322	-3332615.78	-3332462.76
$F_3Al\text{-}OCH(CF_3)_2$	-1330.73	-3493842.16	190.84	0.51938	-3493803.69	-3493648.84
$F_3Al\text{-}OC(CF_3)_3$	-1667.54	-4378133.90	210.33	0.58011	-4378094.05	-4377921.09
$F_3Al\text{-}OC_5F_4N$	-1261.45	-3311941.87	186.76	0.51592	-3311906.45	-3311752.63
$F_3Al\text{-}OTeF_5$	-1124.17	-2951516.74	96.88	0.50788	-2951568.80	-2951417.38
$F_3Al\text{-}OC_{10}F_{15}$	-2494.63	-6549653.24	377.05	0.71498	-6549486.88	-6549273.71
$F_3Al\text{-}C_2F_5$	-1117.03	-2932770.99	116.43	0.46022	-2932789.30	-2932652.08

Table S- 7: Summary of thermodynamic data calculated at the MP2/def-TZVPP level of theory (298.15 K) for the calculation of the non isodesmic reaction:

	E_{SCF} / H	E_{SCF} / kJ·mol^{-1}	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	$G°$ / kJ·mol^{-1}	$H°$ / kJ·mol^{-1}
AlF_3	-541.44	-1421539.65	32.03	0.28443	-1421589.95	-1421505.15
$F_3Al\text{-}C_6F_5$	-1268.34	-3330018.64	191.93	0.47482	-3329965.80	-3329824.23
$F_3Al\text{-}OCH(CF_3)_2$	-1329.83	-3491478.90	201.91	0.47587	-3491416.39	-3491274.51
$F_3Al\text{-}OC(CF_3)_3$	-1666.47	-4375322.82	222.03	0.53039	-4375256.45	-4375098.32
$F_3Al\text{-}OC_5F_4N$	-1260.44	-3309283.57	195.18	0.47019	-3309226.10	-3309085.91
$F_3Al\text{-}OTeF_5$	-1123.48	-2949684.90	101.56	0.45811	-2949717.45	-2949580.86
$F_3Al\text{-}OC_{10}F_{15}$	-2492.98	-6545326.08	404.30	0.64699	-6545112.21	-6544919.31
$F_3Al\text{-}C_2F_5$	-1116.28	-2930783.49	121.46	0.42879	-2930787.39	-2930659.55
$C_6F_5^-$	-726.78	-1908163.79	148.93	0.36871	-1908122.31	-1908012.38
$CH(CF_3)_2O^-$	-788.26	-2069563.47	156.90	0.37197	-2069515.00	-2069404.10
$C(CF_3)_3O^-$	-1124.91	-2953461.47	178.49	0.42887	-2953408.37	-2953280.51
$NC_5F_4O^-$	-718.89	-1887455.63	153.84	0.36465	-1887408.03	-1887299.31
TeF_5O^-	-581.94	-1527872.68	59.90	0.35464	-1527916.04	-1527810.30
$C_{10}F_{15}O^-$	-1951.43	-5123486.33	360.57	0.54462	-5123285.66	-5123123.28
$C_2F_5^-$	-574.71	-1508892.74	77.75	0.32416	-1508909.16	-1508812.51

Table S- 8: Final table for the calculation of the Ligand affinity:

	$\Delta H_R°$ reaction 1 / kJ·mol^{-1}	$\Delta H_R°$ reaction 2 / kJ·mol^{-1}	Ligand Affinity (LA)
	$M(L)_n^- + AlF_3 \rightarrow M(L)_{n-1} + F_3Al\text{-}L^-$	$F_3Al\text{-}L^- \rightarrow AlF_3 + L^-$	Sum of both reactions
	BP86(D3BJ)/def-SV(P)	MP2/def-TZVPP	kJ·mol^{-1}
$[B(OCH(CF_3)_2)_4]^-$	-64.73	365.27	301
$[B(C_6F_5)_4]^-$	22.60	306.71	329
$[Ga(C_2F_5)_4]^-$	58.80	341.89	401
$[B(OC_5F_4N)_4]^-$	-18.07	281.46	263
$[Al(OC(CF_3)_3)_4]^-$	39.26	312.66	352
$[Al(C_6F_5)_4]^-$	60.40	306.71	367
$[Al(OTeF_5)_4]^-$	27.53	265.41	293
$[Ga(OTeF_5)_4]^-$	45.37	265.41	311
$[Al(OC_5F_4N)_4]^-$	70.34	281.46	352
$[Al(OC_{10}F_{15})_4]^-$	87.77	290.88	379

Note: The values on PBEP86 level of theory are shown in Table S- 5 on page 77.

Detailed results for the calculation of the ligand affinity LA and population analysis of the anions

Note: The detailed results for the Lewis acids in Table S- 6 were already mentioned in the previous chapter (calculating the FIA pages 79-123) with exception for AlF_3 and therefore are not listed again. Some molecules were calculated on BP86(D3BJ)/def-SV(P) as well as on MP2/def-TZVPP level of theory. In these cases both results are listed below. Population analysis of the anions for calculation of the charges q_{neg} and q_{surf} (most negatively charged atom and most negatively charged surface atom) were carried out with $pop paboon in turbomole. The atomic charges were obtained with multicenter corrections.

$[Al(C_6F_5)_4]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: s4

Cartesian coordinates in Ångström:
C    -0.6278090   -3.6355285   -2.3466534
C    -0.1138130   -2.6983571   -1.4326692
C    -0.6784127   -1.4346642   -1.2411940
C    -1.7880558   -1.1324154   -2.0362168
C    -2.3459377   -2.0263366   -2.9630895
C    -1.7509490   -3.2900732   -3.1151620
F     0.9828382   -3.0773659   -0.7381841
F    -0.0627595   -4.8469643   -2.5066800
F    -2.2563523   -4.1688668   -3.9980303
F    -3.4196826   -1.7010481   -3.7065003
F    -2.3774999    0.0833009   -1.9260989
C     1.1324154   -1.7880558    2.0362168
C     3.6355285   -0.6278090    2.3466534
C     1.4346642   -0.6784127    1.2411940
C     2.6983571   -0.1138130    1.4326692
C     3.2900732   -1.7509490    3.1151620
C     2.0263366   -2.3459377    2.9630895
F    -0.0833009   -2.3774999    1.9260989
F     4.8469643   -0.0627595    2.5066800
F     1.7010481   -3.4196826    3.7065003
F     4.1688668   -2.2563523    3.9980303
F     3.0773659    0.9828382    0.7381841
C    -2.6983571    0.1138130    1.4326692
C    -2.0263366    2.3459377    2.9630895
C    -1.4346642    0.6784127    1.2411940
C    -1.1324154    1.7880558    2.0362168
C    -3.2900732    1.7509490    3.1151620
C    -3.6355285    0.6278090    2.3466534
F    -3.0773659   -0.9828382    0.7381841
F    -1.7010481    3.4196826    3.7065003
F    -4.8469643    0.0627595    2.5066800
F    -4.1688668    2.2563523    3.9980303
F     0.0833009    2.3774999    1.9260989
Al   -0.0000000   -0.0000000    0.0000000
F     2.2563523    4.1688668   -3.9980303
F     0.0627595    4.8469643   -2.5066800
C     1.7509490    3.2900732   -3.1151620
C     0.6278090    3.6355285   -2.3466534
F     3.4196826    1.7010481   -3.7065003
C     2.3459377    2.0263366   -2.9630895
C     0.1138130    2.6983571   -1.4326692
C     1.7880558    1.1324154   -2.0362168
F    -0.9828382    3.0773659   -0.7381841
C     0.6784127    1.4346642   -1.2411940
F     2.3774999   -0.0833009   -1.9260989

SCF energy GEOOPT =  -3151.863922955 H
ZPE =   504.8 kJ/mol
FREEH energy =   613.86 kJ/mol
```

```
FREEH entropy =   1.05443 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   169.    84 e     -0.12319426 H =     -3.35229 eV
   LUMO:   170.    43 b     +0.03433182 H =     +0.93422 eV
   Gap :                    +0.15752608 H =     +4.28650 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol          IR     RAMAN
     1                      -0.00         0.00000         -       -
     2                      -0.00         0.00000         -       -
     3                      -0.00         0.00000         -       -
     4                       0.00         0.00000         -       -
     5                       0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
     7        b             16.65         0.00000       YES     YES
     8        b             18.69         0.00774       YES     YES
     9        b             19.77         0.00000       YES     YES
    10        b             24.40         0.03282       YES     YES
    11        e             27.31         0.00061       YES     YES
    12        e             27.31         0.00061       YES     YES
    13        e             32.33         0.01306       YES     YES
    14        e             32.33         0.01306       YES     YES
    15        b             42.72         0.00906       YES     YES
    16        e             83.38         0.02662       YES     YES
    17        e             83.38         0.02662       YES     YES
    18        b             85.15         0.00000       YES     YES
    19        b             98.83         0.05061       YES     YES
    20        b            106.97         0.00000       YES     YES
    21        e            108.54         0.36831       YES     YES
    22        e            108.54         0.36830       YES     YES
    23        b            109.29         0.97395       YES     YES
    24        a            122.50         0.00000       NO      YES
    25        e            127.37         0.03922       YES     YES
    26        e            127.37         0.03922       YES     YES
    27        b            128.55         0.00000       YES     YES
    28        b            131.48         0.06216       YES     YES
    29        e            154.66         0.01021       YES     YES
    30        e            154.66         0.01021       YES     YES
    31        b            156.58         0.08506       YES     YES
    32        b            158.73         0.00000       YES     YES
    33        e            215.35         0.60730       YES     YES
    34        e            215.35         0.60730       YES     YES
    35        b            221.59         0.00000       YES     YES
    36        b            221.93         1.64313       YES     YES
    37        e            264.67         0.40149       YES     YES
    38        e            264.67         0.40149       YES     YES
    39        b            265.01         0.08534       YES     YES
    40        b            265.17         0.00000       YES     YES
    41        b            266.66         0.91139       YES     YES
    42        e            267.09         0.18899       YES     YES
    43        e            267.09         0.18899       YES     YES
    44        a            269.38         0.00000       NO      YES
    45        e            304.16         4.41949       YES     YES
    46        e            304.16         4.41947       YES     YES
    47        b            304.32         0.00000       YES     YES
    48        b            305.18         1.75289       YES     YES
    49        e            315.65        11.55817       YES     YES
    50        e            315.65        11.55814       YES     YES
    51        b            321.05        25.86839       YES     YES
    52        a            343.70         0.00000       NO      YES
    53        e            347.99         2.35376       YES     YES
    54        e            347.99         2.35375       YES     YES
    55        b            354.23         0.01608       YES     YES
    56        a            361.87         0.00000       NO      YES
    57        e            388.19        43.62108       YES     YES
    58        e            388.19        43.62109       YES     YES
    59        b            399.90         2.21439       YES     YES
    60        e            400.01         0.07178       YES     YES
```

61	e	400.01	0.07179	YES	YES
62	b	400.10	0.00000	YES	YES
63	b	405.31	57.84463	YES	YES
64	a	432.87	0.00000	NO	YES
65	e	434.31	0.59232	YES	YES
66	e	434.31	0.59232	YES	YES
67	b	434.41	0.68900	YES	YES
68	a	475.66	0.00000	NO	YES
69	e	483.01	1.58745	YES	YES
70	e	483.01	1.58749	YES	YES
71	b	485.10	3.54530	YES	YES
72	b	486.96	0.00000	YES	YES
73	e	491.92	20.73944	YES	YES
74	e	491.92	20.73943	YES	YES
75	b	496.36	49.22281	YES	YES
76	e	563.82	0.02787	YES	YES
77	e	563.82	0.02787	YES	YES
78	b	563.85	0.00000	YES	YES
79	b	564.00	0.28300	YES	YES
80	e	598.76	11.24112	YES	YES
81	e	598.76	11.24112	YES	YES
82	a	606.19	0.00000	NO	YES
83	b	613.07	48.56970	YES	YES
84	e	630.70	0.19321	YES	YES
85	e	630.70	0.19321	YES	YES
86	b	631.43	0.00000	YES	YES
87	b	632.25	2.31903	YES	YES
88	a	728.82	0.00000	NO	YES
89	e	735.91	3.47938	YES	YES
90	e	735.91	3.47938	YES	YES
91	b	737.56	1.67334	YES	YES
92	a	775.29	0.00000	NO	YES
93	e	789.76	3.85949	YES	YES
94	e	789.76	3.85949	YES	YES
95	b	797.52	2.10258	YES	YES
96	a	957.98	0.00000	NO	YES
97	e	964.81	293.46664	YES	YES
98	e	964.81	293.46666	YES	YES
99	b	965.61	25.73607	YES	YES
100	e	1071.59	296.44134	YES	YES
101	e	1071.59	296.44132	YES	YES
102	b	1073.02	468.51554	YES	YES
103	b	1074.66	0.00000	YES	YES
104	a	1123.90	0.00000	NO	YES
105	b	1130.74	0.41554	YES	YES
106	e	1131.52	3.87007	YES	YES
107	e	1131.52	3.87008	YES	YES
108	e	1258.91	47.43622	YES	YES
109	e	1258.91	47.43625	YES	YES
110	b	1259.46	75.96522	YES	YES
111	a	1261.43	0.00000	NO	YES
112	b	1359.77	23.88304	YES	YES
113	e	1359.91	28.12823	YES	YES
114	e	1359.91	28.12821	YES	YES
115	a	1363.01	0.00000	NO	YES
116	e	1366.90	9.11007	YES	YES
117	e	1366.90	9.11007	YES	YES
118	b	1371.39	12.64006	YES	YES
119	a	1378.11	0.00000	NO	YES
120	a	1450.87	0.00000	NO	YES
121	b	1465.70	108.89222	YES	YES
122	e	1466.96	878.76745	YES	YES
123	e	1466.96	878.76745	YES	YES
124	e	1507.41	164.41510	YES	YES
125	e	1507.41	164.41509	YES	YES
126	b	1507.57	305.73877	YES	YES
127	a	1510.40	0.00000	NO	YES
128	b	1618.18	0.00000	YES	YES
129	e	1620.12	11.67413	YES	YES
130	e	1620.12	11.67436	YES	YES

```
   131        b           1620.34        22.82239       YES     YES
   132        e           1624.13        50.53252       YES     YES
   133        e           1624.13        50.53277       YES     YES
   134        b           1624.47        66.55497       YES     YES
   135        b           1625.05         0.00000       YES     YES
$end
```

atom	charge
1 c	0.1758
2 c	0.2283
3 c	-0.1942
4 c	0.2129
5 c	0.1800
6 c	0.1513
7 f	-0.1856
8 f	-0.2115
9 f	-0.1842
10 f	-0.2121
11 f	-0.1718
12 c	0.2129
13 c	0.1758
14 c	-0.1942
15 c	0.2283
16 c	0.1513
17 c	0.1800
18 f	-0.1718
19 f	-0.2115
20 f	-0.2121
21 f	-0.1842
22 f	-0.1856
23 c	0.2283
24 c	0.1800
25 c	-0.1942
26 c	0.2129
27 c	0.1513
28 c	0.1758
29 f	-0.1856
30 f	-0.2121
31 f	-0.2115
32 f	-0.1842
33 f	-0.1718
34 al	-0.1560
35 f	-0.1842
36 f	-0.2115
37 c	0.1513
38 c	0.1758
39 f	-0.2121
40 c	0.1800
41 c	0.2283
42 c	0.2129
43 f	-0.1856
44 c	-0.1942
45 f	-0.1718

$[B(C_6F_5)_4]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: s4

Cartesian coordinates in Ångström:
C     1.4893097    2.9527292    2.3009610
C     1.3797677    1.9481326    1.3210745
C     0.1842580    1.2649211    1.0475905
C    -0.9001080    1.6295071    1.8666279
```

```
C    -0.8417172    2.6244254    2.8531628
C     0.3727012    3.2917438    3.0754988
F     2.5201453    1.6765385    0.6537900
F     2.6611619    3.5811648    2.5124046
F     0.4640423    4.2458216    4.0195856
F    -1.9230068    2.9390851    3.5905742
F    -2.0929389    1.0135116    1.7151650
C     1.6295071    0.9001080   -1.8666279
C     2.9527292   -1.4893097   -2.3009610
C     1.2649211   -0.1842580   -1.0475905
C     1.9481326   -1.3797677   -1.3210745
C     3.2917438   -0.3727012   -3.0754988
C     2.6244254    0.8417172   -2.8531628
F     1.0135116    2.0929389   -1.7151650
F     3.5811648   -2.6611619   -2.5124046
F     2.9390851    1.9230068   -3.5905742
F     4.2458216   -0.4640423   -4.0195856
F     1.6765385   -2.5201453   -0.6537900
C    -1.9481326    1.3797677   -1.3210745
C    -2.6244254   -0.8417172   -2.8531628
C    -1.2649211    0.1842580   -1.0475905
C    -1.6295071   -0.9001080   -1.8666279
C    -3.2917438    0.3727012   -3.0754988
C    -2.9527292    1.4893097   -2.3009610
F    -1.6765385    2.5201453   -0.6537900
F    -2.9390851   -1.9230068   -3.5905742
F    -3.5811648    2.6611619   -2.5124046
F    -4.2458216    0.4640423   -4.0195856
F    -1.0135116   -2.0929389   -1.7151650
B     0.0000000   -0.0000000    0.0000000
F    -0.4640423   -4.2458216    4.0195856
F    -2.6611619   -3.5811648    2.5124046
C    -0.3727012   -3.2917438    3.0754988
C    -1.4893097   -2.9527292    2.3009610
F     1.9230068   -2.9390851    3.5905742
C     0.8417172   -2.6244254    2.8531628
C    -1.3797677   -1.9481326    1.3210745
C     0.9001080   -1.6295071    1.8666279
F    -2.5201453   -1.6765385    0.6537900
C    -0.1842580   -1.2649211    1.0475905
F     2.0929389   -1.0135116    1.7151650

SCF energy GEOOPT =  -2934.289237671 H
ZPE =   520.9 kJ/mol
FREEH energy =   624.23 kJ/mol
FREEH entropy =   0.97863 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   165.    82 e     -0.11415747 H =     -3.10638 eV
   LUMO:   166.    42 b     +0.04078646 H =     +1.10986 eV
   Gap :                    +0.15494394 H =     +4.21624 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        b             25.56         0.00000       YES     YES
     8        b             26.42         0.01329       YES     YES
     9        b             31.73         0.00000       YES     YES
    10        b             32.82         0.01257       YES     YES
    11        e             40.81         0.01061       YES     YES
    12        e             40.81         0.01061       YES     YES
    13        e             51.24         0.01467       YES     YES
    14        e             51.25         0.01467       YES     YES
    15        b             60.34         0.00112       YES     YES
```

16	e	110.32	0.01255	YES	YES
17	e	110.32	0.01255	YES	YES
18	b	121.82	0.15753	YES	YES
19	b	126.65	0.00000	YES	YES
20	b	128.00	0.00000	YES	YES
21	b	132.37	0.00000	YES	YES
22	e	138.84	0.01312	YES	YES
23	e	138.84	0.01312	YES	YES
24	b	143.47	0.00154	YES	YES
25	e	147.43	0.06835	YES	YES
26	e	147.43	0.06835	YES	YES
27	b	154.62	0.00000	YES	YES
28	b	161.28	0.02681	YES	YES
29	e	167.02	0.09029	YES	YES
30	e	167.02	0.09029	YES	YES
31	b	167.06	0.16482	YES	YES
32	a	176.75	0.00000	NO	YES
33	e	232.63	1.56875	YES	YES
34	e	232.63	1.56875	YES	YES
35	b	240.76	0.00000	YES	YES
36	b	242.97	4.13787	YES	YES
37	e	262.16	0.11514	YES	YES
38	e	262.16	0.11514	YES	YES
39	b	262.23	0.00000	YES	YES
40	b	262.37	0.02109	YES	YES
41	e	273.14	0.03854	YES	YES
42	e	273.14	0.03854	YES	YES
43	b	273.58	0.06166	YES	YES
44	b	274.34	0.00000	YES	YES
45	b	309.01	0.00000	YES	YES
46	b	310.51	0.01039	YES	YES
47	e	310.62	0.77797	YES	YES
48	e	310.62	0.77796	YES	YES
49	e	339.65	1.22056	YES	YES
50	e	339.65	1.22056	YES	YES
51	b	345.06	7.38130	YES	YES
52	b	351.48	0.00000	YES	YES
53	e	366.08	0.46634	YES	YES
54	e	366.08	0.46633	YES	YES
55	b	390.83	0.30916	YES	YES
56	e	391.71	0.21522	YES	YES
57	e	391.71	0.21522	YES	YES
58	b	392.88	0.00000	YES	YES
59	b	394.17	2.19377	YES	YES
60	a	410.87	0.00000	NO	YES
61	b	435.33	0.00000	YES	YES
62	e	436.43	0.01351	YES	YES
63	e	436.43	0.01351	YES	YES
64	b	436.92	0.17180	YES	YES
65	b	462.78	1.04887	YES	YES
66	e	465.41	0.98642	YES	YES
67	e	465.41	0.98642	YES	YES
68	a	481.10	0.00000	NO	YES
69	b	518.56	0.40716	YES	YES
70	e	519.96	0.08756	YES	YES
71	e	519.96	0.08756	YES	YES
72	b	522.73	0.00000	YES	YES
73	b	563.77	4.39569	YES	YES
74	e	565.58	2.19500	YES	YES
75	e	565.58	2.19499	YES	YES
76	a	567.61	0.00000	NO	YES
77	e	601.83	11.06068	YES	YES
78	e	601.83	11.06066	YES	YES
79	b	605.44	23.38878	YES	YES
80	e	630.42	0.44569	YES	YES
81	e	630.42	0.44569	YES	YES
82	b	630.45	0.00000	YES	YES
83	b	633.11	0.13669	YES	YES
84	e	672.80	34.35898	YES	YES
85	e	672.80	34.35888	YES	YES

86	a	676.67	0.00000	NO	YES
87	b	723.74	107.55176	YES	YES
88	a	738.56	0.00000	NO	YES
89	b	756.52	10.85905	YES	YES
90	e	764.08	29.16302	YES	YES
91	e	764.08	29.16310	YES	YES
92	a	818.03	0.00000	NO	YES
93	e	914.26	0.24487	YES	YES
94	e	914.26	0.24487	YES	YES
95	b	962.07	22.18167	YES	YES
96	b	965.50	0.00000	YES	YES
97	b	982.30	39.00817	YES	YES
98	e	987.46	337.91666	YES	YES
99	e	987.46	337.91658	YES	YES
100	a	1088.15	0.00000	NO	YES
101	e	1089.69	147.48640	YES	YES
102	e	1089.69	147.48633	YES	YES
103	b	1107.48	377.59336	YES	YES
104	a	1126.48	0.00000	NO	YES
105	b	1135.70	9.85601	YES	YES
106	e	1137.31	5.11933	YES	YES
107	e	1137.31	5.11931	YES	YES
108	e	1269.78	23.57198	YES	YES
109	e	1269.78	23.57200	YES	YES
110	b	1275.14	85.03035	YES	YES
111	b	1275.31	0.00000	YES	YES
112	a	1349.48	0.00000	NO	YES
113	e	1353.78	6.21845	YES	YES
114	e	1353.78	6.21848	YES	YES
115	b	1354.86	4.58823	YES	YES
116	e	1378.31	14.56231	YES	YES
117	e	1378.31	14.56240	YES	YES
118	b	1388.74	6.33662	YES	YES
119	b	1393.43	0.00000	YES	YES
120	a	1453.33	0.00000	NO	YES
121	b	1470.99	73.35057	YES	YES
122	e	1472.63	703.64391	YES	YES
123	e	1472.63	703.64383	YES	YES
124	e	1511.96	184.88432	YES	YES
125	e	1511.96	184.88432	YES	YES
126	b	1513.25	366.33350	YES	YES
127	a	1517.32	0.00000	NO	YES
128	b	1616.59	0.00000	YES	YES
129	e	1619.08	6.56670	YES	YES
130	e	1619.08	6.56665	YES	YES
131	b	1620.58	11.22745	YES	YES
132	e	1630.17	33.89311	YES	YES
133	e	1630.17	33.89303	YES	YES
134	b	1630.57	57.14844	YES	YES
135	a	1633.05	0.00000	NO	YES

$end

atom	charge
1 c	0.1679
2 c	0.2259
3 c	0.0253
4 c	0.2450
5 c	0.1733
6 c	0.1433
7 f	-0.1873
8 f	-0.2207
9 f	-0.1995
10 f	-0.2247
11 f	-0.1606
12 c	0.2450
13 c	0.1679

14	c	0.0253
15	c	0.2259
16	c	0.1433
17	c	0.1733
18	f	-0.1606
19	f	-0.2207
20	f	-0.2247
21	f	-0.1995
22	f	-0.1873
23	c	0.2259
24	c	0.1733
25	c	0.0253
26	c	0.2450
27	c	0.1433
28	c	0.1679
29	f	-0.1873
30	f	-0.2247
31	f	-0.2207
32	f	-0.1995
33	f	-0.1606
34	b	-0.9516
35	f	-0.1995
36	f	-0.2207
37	c	0.1433
38	c	0.1679
39	f	-0.2247
40	c	0.1733
41	c	0.2259
42	c	0.2450
43	f	-0.1873
44	c	0.0253
45	f	-0.1606

$[B(OCH(CF_3)_2)_4]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: s4

Cartesian coordinates in Ångström:

B	0.0000000	0.0000000	0.0000000
O	1.0803978	0.6007831	-0.8050745
O	0.6007831	-1.0803978	0.8050745
O	-0.6007831	1.0803978	0.8050745
C	1.0419688	1.9267045	-1.1770279
C	0.8829651	2.0464864	-2.7064992
C	2.3114777	2.6313097	-0.6526010
F	-0.2900925	1.5124579	-3.0980473
F	1.8697308	1.4182534	-3.3803337
F	0.8848391	3.3495146	-3.1059830
F	2.3012832	3.9644865	-0.9078477
F	3.4479020	2.1248417	-1.1868252
F	2.3997202	2.4802337	0.6882395
H	0.1828170	2.4707606	-0.7232269
C	1.9267045	-1.0419688	1.1770279
C	2.6313097	-2.3114777	0.6526010
C	2.0464864	-0.8829651	2.7064992
C	-1.9267045	1.0419688	1.1770279
C	-2.6313097	2.3114777	0.6526010
C	-2.0464864	0.8829651	2.7064992
F	1.5124579	0.2900925	3.0980473
F	1.4182534	-1.8697308	3.3803337
F	3.3495146	-0.8848391	3.1059830
F	3.9644865	-2.3012832	0.9078477
F	2.1248417	-3.4479020	1.1868252
F	2.4802337	-2.3997202	-0.6882395
F	-1.5124579	-0.2900925	3.0980473
F	-3.3495146	0.8848391	3.1059830

```
F    -1.4182534    1.8697308    3.3803337
F    -3.9644865    2.3012832    0.9078477
F    -2.1248417    3.4479020    1.1868252
F    -2.4802337    2.3997202   -0.6882395
H     2.4707606   -0.1828170    0.7232269
H    -2.4707606    0.1828170    0.7232269
F    -0.8848391   -3.3495146   -3.1059830
F    -2.3012832   -3.9644865   -0.9078477
H    -0.1828170   -2.4707606   -0.7232269
F    -2.3997202   -2.4802337    0.6882395
C    -1.0419688   -1.9267045   -1.1770279
C    -2.3114777   -2.6313097   -0.6526010
C    -0.8829651   -2.0464864   -2.7064992
F     0.2900925   -1.5124579   -3.0980473
O    -1.0803978   -0.6007831   -0.8050745
F    -1.8697308   -1.4182534   -3.3803337
F    -3.4479020   -2.1248417   -1.1868252

SCF energy GEOOPT =  -3179.829831888 H
ZPE =   548.4 kJ/mol
FREEH energy =   652.36 kJ/mol
FREEH entropy =   1.07771 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   165.    82 e     -0.12382869 H =     -3.36955 eV
   LUMO:   166.    43 a     +0.13731274 H =     +3.73647 eV
   Gap :                    +0.26114143 H =     +7.10602 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        e             13.17         0.04458       YES     YES
     8        e             13.17         0.04458       YES     YES
     9        b             13.84         0.00503       YES     YES
    10        b             14.68         0.00000       YES     YES
    11        b             22.25         0.00000       YES     YES
    12        e             29.73         0.02635       YES     YES
    13        e             29.73         0.02635       YES     YES
    14        b             30.02         0.08100       YES     YES
    15        e             34.41         0.23937       YES     YES
    16        e             34.41         0.23937       YES     YES
    17        b             34.87         0.01049       YES     YES
    18        b             37.31         0.00000       YES     YES
    19        b             41.48         0.30872       YES     YES
    20        e             62.14         0.03437       YES     YES
    21        e             62.14         0.03437       YES     YES
    22        a             66.94         0.00000       NO      YES
    23        b             76.91         0.10156       YES     YES
    24        e             88.23         0.09705       YES     YES
    25        e             88.23         0.09705       YES     YES
    26        a            106.30         0.00000       NO      YES
    27        b            112.05         0.00000       YES     YES
    28        b            112.57         0.38118       YES     YES
    29        e            155.72         2.66356       YES     YES
    30        e            155.72         2.66355       YES     YES
    31        b            169.46         0.00000       YES     YES
    32        b            170.90         0.27010       YES     YES
    33        e            198.19         0.10153       YES     YES
    34        e            198.19         0.10153       YES     YES
    35        a            203.87         0.00000       NO      YES
    36        b            216.19         0.89287       YES     YES
    37        e            257.84         0.75500       YES     YES
    38        e            257.84         0.75500       YES     YES
    39        b            275.18         2.24238       YES     YES
```

40	a	284.44	0.00000	NO	YES
41	e	285.89	0.10722	YES	YES
42	e	285.89	0.10722	YES	YES
43	b	286.12	0.17343	YES	YES
44	b	286.75	0.00000	YES	YES
45	b	318.39	0.73980	YES	YES
46	e	318.40	1.33846	YES	YES
47	e	318.40	1.33846	YES	YES
48	a	322.14	0.00000	NO	YES
49	e	342.35	0.01083	YES	YES
50	e	342.35	0.01083	YES	YES
51	b	349.26	0.56494	YES	YES
52	e	380.20	3.59295	YES	YES
53	e	380.20	3.59294	YES	YES
54	a	407.07	0.00000	NO	YES
55	a	425.05	0.00000	NO	YES
56	b	461.79	0.17853	YES	YES
57	e	501.21	0.85646	YES	YES
58	e	501.21	0.85645	YES	YES
59	b	509.40	19.19411	YES	YES
60	a	513.60	0.00000	NO	YES
61	b	519.36	6.24236	YES	YES
62	b	519.51	0.00000	YES	YES
63	e	519.52	2.05086	YES	YES
64	e	519.52	2.05085	YES	YES
65	b	524.28	0.02446	YES	YES
66	e	527.95	9.55655	YES	YES
67	e	527.95	9.55653	YES	YES
68	b	534.12	2.03447	YES	YES
69	e	534.23	0.55555	YES	YES
70	e	534.23	0.55556	YES	YES
71	b	534.83	0.00000	YES	YES
72	a	546.18	0.00000	NO	YES
73	b	617.47	22.10049	YES	YES
74	e	643.58	30.94048	YES	YES
75	e	643.58	30.94047	YES	YES
76	a	667.67	0.00000	NO	YES
77	e	667.81	27.36863	YES	YES
78	e	667.81	27.36873	YES	YES
79	b	671.73	108.10415	YES	YES
80	a	703.68	0.00000	NO	YES
81	b	723.71	6.61588	YES	YES
82	e	727.14	7.85019	YES	YES
83	e	727.14	7.85018	YES	YES
84	a	789.72	0.00000	NO	YES
85	e	852.86	51.58579	YES	YES
86	e	852.86	51.58577	YES	YES
87	b	858.33	53.85282	YES	YES
88	a	866.87	0.00000	NO	YES
89	b	878.46	0.00000	YES	YES
90	e	878.61	11.48661	YES	YES
91	e	878.61	11.48682	YES	YES
92	b	880.81	62.30526	YES	YES
93	b	971.39	210.10723	YES	YES
94	e	1031.93	310.37604	YES	YES
95	e	1031.93	310.37629	YES	YES
96	b	1086.11	0.00004	YES	YES
97	b	1086.15	346.10787	YES	YES
98	e	1088.27	86.39810	YES	YES
99	e	1088.27	86.39806	YES	YES
100	e	1121.67	69.07625	YES	YES
101	e	1121.67	69.07626	YES	YES
102	a	1126.80	0.00000	NO	YES
103	b	1135.51	68.38521	YES	YES
104	e	1165.28	28.47490	YES	YES
105	e	1165.28	28.47445	YES	YES
106	a	1165.50	0.00000	NO	YES
107	b	1172.20	74.96651	YES	YES
108	b	1177.61	158.36142	YES	YES
109	e	1180.75	1222.00959	YES	YES

110	e	1180.75	1222.00884	YES	YES
111	b	1213.38	585.80252	YES	YES
112	e	1215.63	594.59102	YES	YES
113	e	1215.63	594.59243	YES	YES
114	a	1215.83	0.00000	NO	YES
115	a	1228.32	0.00000	NO	YES
116	e	1238.98	77.88765	YES	YES
117	e	1238.98	77.88626	YES	YES
118	b	1239.81	0.00000	YES	YES
119	b	1242.68	294.93568	YES	YES
120	b	1270.34	0.00000	YES	YES
121	e	1277.26	228.85816	YES	YES
122	e	1277.26	228.85852	YES	YES
123	b	1280.16	54.06044	YES	YES
124	b	1328.42	0.00000	YES	YES
125	e	1331.42	1.58830	YES	YES
126	e	1331.42	1.58841	YES	YES
127	b	1341.06	42.39842	YES	YES
128	b	1357.68	0.00000	YES	YES
129	e	1363.10	70.85195	YES	YES
130	e	1363.10	70.85142	YES	YES
131	b	1366.98	206.88522	YES	YES
132	e	2975.78	34.86472	YES	YES
133	e	2975.78	34.86471	YES	YES
134	b	2975.81	20.56211	YES	YES
135	b	2976.27	0.00000	YES	YES

$end

atom	charge
1 b	-0.1992
2 o	-0.1503
3 o	-0.1503
4 o	-0.1503
5 c	-0.0609
6 c	0.5558
7 c	0.5610
8 f	-0.1748
9 f	-0.1882
10 f	-0.2125
11 f	-0.2028
12 f	-0.1962
13 f	-0.1834
14 h	0.0521
15 c	-0.0609
16 c	0.5610
17 c	0.5558
18 c	-0.0609
19 c	0.5610
20 c	0.5558
21 f	-0.1748
22 f	-0.1882
23 f	-0.2125
24 f	-0.2028
25 f	-0.1962
26 f	-0.1834
27 f	-0.1748
28 f	-0.2125
29 f	-0.1882
30 f	-0.2028
31 f	-0.1962
32 f	-0.1834
33 h	0.0521
34 h	0.0521
35 f	-0.2125
36 f	-0.2028
37 h	0.0521

```
                    38 f   |   -0.1834
                    39 c   |   -0.0609
                    40 c   |    0.5610
                    41 c   |    0.5558
                    42 f   |   -0.1748
                    43 o   |   -0.1503
                    44 f   |   -0.1882
                    45 f   |   -0.1962
                  -------------------------
```

$[Al(OC(CF_3)_3)_4]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: s4

Cartesian coordinates in Ångström:
Al    0.0000000   -0.0000000    0.0000000
F    -3.0318554    0.2835492   -2.8010363
F    -1.3017983   -0.5233695   -3.8393431
F    -3.1714460   -1.6490024   -3.7991377
F    -3.4518196   -3.3803642   -1.6507739
F    -4.1876720   -1.4211006   -1.0380896
F    -2.8155783   -2.5093424    0.2473285
F     0.3980426   -2.0380367   -2.2716481
F    -1.1078741   -3.3315586   -3.1781520
F    -0.6538372   -3.4993708   -1.0540349
O    -1.3936644   -0.5604766   -0.9199578
C    -0.7956366   -2.6220052   -2.0673923
C    -2.3603431   -0.8461888   -3.0669893
C    -3.1028286   -2.2243431   -1.0299070
C    -1.8775625   -1.5254099   -1.7295068
F     0.2835492    3.0318554    2.8010363
F     3.0318554   -0.2835492   -2.8010363
F    -0.2835492   -3.0318554    2.8010363
F    -0.5233695    1.3017983    3.8393431
F     1.3017983    0.5233695   -3.8393431
F     0.5233695   -1.3017983    3.8393431
F    -1.6490024    3.1714460    3.7991377
F     3.1714460    1.6490024   -3.7991377
F     1.6490024   -3.1714460    3.7991377
F    -3.3803642    3.4518196    1.6507739
F     3.4518196    3.3803642   -1.6507739
F     3.3803642   -3.4518196    1.6507739
F    -1.4211006    4.1876720    1.0380896
F     4.1876720    1.4211006   -1.0380896
F     1.4211006   -4.1876720    1.0380896
F    -2.5093424    2.8155783   -0.2473285
F     2.8155783    2.5093424    0.2473285
F     2.5093424   -2.8155783   -0.2473285
F    -2.0380367   -0.3980426    2.2716481
F    -0.3980426    2.0380367   -2.2716481
F     2.0380367    0.3980426    2.2716481
F    -3.3315586    1.1078741    3.1781520
F     1.1078741    3.3315586   -3.1781520
F     3.3315586   -1.1078741    3.1781520
F    -3.4993708    0.6538372    1.0540349
F     0.6538372    3.4993708   -1.0540349
F     3.4993708   -0.6538372    1.0540349
O    -0.5604766    1.3936644    0.9199578
O     1.3936644    0.5604766   -0.9199578
O     0.5604766   -1.3936644    0.9199578
C    -2.6220052    0.7956366    2.0673923
C     0.7956366    2.6220052   -2.0673923
C     2.6220052   -0.7956366    2.0673923
C    -0.8461888    2.3603431    3.0669893
C     2.3603431    0.8461888   -3.0669893
C     0.8461888   -2.3603431    3.0669893
C    -2.2243431    3.1028286    1.0299070
```

```
C     3.1028286    2.2243431   -1.0299070
C     2.2243431   -3.1028286    1.0299070
C    -1.5254099    1.8775625    1.7295068
C     1.8775625    1.5254099   -1.7295068
C     1.5254099   -1.8775625    1.7295068

SCF energy GEOOPT =  -4744.673250758 H
ZPE =   575.2 kJ/mol
FREEH energy =   721.13 kJ/mol
FREEH entropy =   1.33929 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   233.   116 e     -0.15111313 H =     -4.11200 eV
   LUMO:   234.    60 a     +0.10085255 H =     +2.74434 eV
   Gap :                    +0.25196568 H =     +6.85634 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        e             14.90         0.00000       YES     YES
     8        e             14.90         0.00000       YES     YES
     9        b             17.22         0.02465       YES     YES
    10        b             21.33         0.00000       YES     YES
    11        b             24.14         0.11889       YES     YES
    12        e             31.43         0.00413       YES     YES
    13        e             31.43         0.00413       YES     YES
    14        a             32.03         0.00000       NO      YES
    15        b             43.59         0.06350       YES     YES
    16        e             44.89         0.05709       YES     YES
    17        e             44.89         0.05709       YES     YES
    18        a             59.09         0.00000       NO      YES
    19        a             61.20         0.00000       NO      YES
    20        b             71.06         0.72890       YES     YES
    21        b             73.81         0.00354       YES     YES
    22        e             74.00         0.04166       YES     YES
    23        e             74.00         0.04166       YES     YES
    24        b             77.27         0.00239       YES     YES
    25        e             77.69         0.18302       YES     YES
    26        e             77.69         0.18302       YES     YES
    27        a             79.31         0.00000       NO      YES
    28        a             80.05         0.00000       NO      YES
    29        e             82.79         0.45566       YES     YES
    30        e             82.79         0.45566       YES     YES
    31        b             88.15         0.01083       YES     YES
    32        a             90.60         0.00000       NO      YES
    33        e             94.75         0.62857       YES     YES
    34        e             94.75         0.62857       YES     YES
    35        b             97.65         1.32279       YES     YES
    36        a            110.95         0.00000       NO      YES
    37        e            153.19         0.48109       YES     YES
    38        e            153.19         0.48109       YES     YES
    39        a            157.72         0.00000       NO      YES
    40        b            159.55         0.06053       YES     YES
    41        e            162.22         1.02701       YES     YES
    42        e            162.22         1.02701       YES     YES
    43        a            163.96         0.00000       NO      YES
    44        b            164.43         1.10831       YES     YES
    45        b            189.58         5.55404       YES     YES
    46        e            193.24         2.97926       YES     YES
    47        e            193.24         2.97926       YES     YES
    48        a            215.82         0.00000       NO      YES
    49        e            262.42         1.14305       YES     YES
    50        e            262.42         1.14305       YES     YES
    51        b            271.13         3.44089       YES     YES
```

52	a	272.23	0.00000	NO	YES
53	e	277.89	3.97711	YES	YES
54	e	277.89	3.97711	YES	YES
55	b	283.51	2.52914	YES	YES
56	a	283.56	0.00000	NO	YES
57	e	284.71	0.03784	YES	YES
58	e	284.71	0.03784	YES	YES
59	b	285.11	0.12510	YES	YES
60	b	285.70	0.00000	YES	YES
61	b	304.12	12.25182	YES	YES
62	e	304.33	8.59729	YES	YES
63	e	304.33	8.59729	YES	YES
64	a	310.72	0.00000	NO	YES
65	e	314.55	0.01921	YES	YES
66	e	314.55	0.01921	YES	YES
67	a	318.70	0.00000	NO	YES
68	b	319.54	1.16277	YES	YES
69	e	322.85	1.04054	YES	YES
70	e	322.85	1.04054	YES	YES
71	b	324.71	1.93166	YES	YES
72	a	326.38	0.00000	NO	YES
73	e	343.29	1.61838	YES	YES
74	e	343.29	1.61838	YES	YES
75	b	349.45	4.62833	YES	YES
76	e	355.14	10.58430	YES	YES
77	e	355.14	10.58430	YES	YES
78	a	355.89	0.00000	NO	YES
79	b	372.13	50.65808	YES	YES
80	a	390.92	0.00000	NO	YES
81	b	434.16	39.26935	YES	YES
82	e	450.06	62.07331	YES	YES
83	e	450.06	62.07330	YES	YES
84	a	516.40	0.00000	NO	YES
85	a	518.51	0.00000	NO	YES
86	e	518.93	3.97843	YES	YES
87	e	518.93	3.97843	YES	YES
88	b	519.47	8.21447	YES	YES
89	a	520.90	0.00000	NO	YES
90	e	520.91	11.74333	YES	YES
91	e	520.91	11.74333	YES	YES
92	b	522.07	6.59957	YES	YES
93	b	524.24	0.19663	YES	YES
94	e	524.31	0.88448	YES	YES
95	e	524.31	0.88448	YES	YES
96	a	527.56	0.00000	NO	YES
97	b	544.67	18.23423	YES	YES
98	e	551.79	13.26018	YES	YES
99	e	551.79	13.26018	YES	YES
100	e	554.27	0.21168	YES	YES
101	e	554.27	0.21168	YES	YES
102	b	554.52	0.46673	YES	YES
103	a	554.79	0.00000	NO	YES
104	b	556.93	0.00000	YES	YES
105	b	557.24	1.61506	YES	YES
106	e	561.71	23.49230	YES	YES
107	e	561.71	23.49229	YES	YES
108	e	707.56	0.92153	YES	YES
109	e	707.56	0.92153	YES	YES
110	a	707.91	0.00000	NO	YES
111	a	709.00	0.00000	NO	YES
112	b	709.16	43.93581	YES	YES
113	e	710.23	88.94851	YES	YES
114	e	710.23	88.94852	YES	YES
115	b	710.27	40.84483	YES	YES
116	a	725.27	0.00000	NO	YES
117	b	736.62	1.28589	YES	YES
118	e	738.39	4.85046	YES	YES
119	e	738.39	4.85046	YES	YES
120	a	778.11	0.00000	NO	YES
121	b	813.95	13.58564	YES	YES

122	e	830.17	26.65696	YES	YES
123	e	830.17	26.65696	YES	YES
124	e	957.58	3.52236	YES	YES
125	e	957.58	3.52236	YES	YES
126	a	958.12	0.00000	NO	YES
127	b	961.60	70.04680	YES	YES
128	a	962.77	0.00000	NO	YES
129	e	965.50	364.26241	YES	YES
130	e	965.50	364.26239	YES	YES
131	b	966.06	239.25263	YES	YES
132	b	1110.83	18.96430	YES	YES
133	e	1113.22	5.97870	YES	YES
134	e	1113.22	5.97871	YES	YES
135	a	1121.13	0.00000	NO	YES
136	e	1132.61	12.53091	YES	YES
137	e	1132.61	12.53091	YES	YES
138	a	1135.20	0.00000	NO	YES
139	a	1139.16	0.00000	NO	YES
140	b	1139.43	30.51715	YES	YES
141	b	1141.70	0.90289	YES	YES
142	e	1143.76	12.52315	YES	YES
143	e	1143.76	12.52315	YES	YES
144	a	1193.78	0.00000	NO	YES
145	e	1198.48	18.67923	YES	YES
146	e	1198.48	18.67923	YES	YES
147	b	1200.61	2.02006	YES	YES
148	a	1203.03	0.00000	NO	YES
149	e	1210.29	3.87515	YES	YES
150	e	1210.29	3.87515	YES	YES
151	b	1214.51	1.58844	YES	YES
152	b	1218.17	938.24895	YES	YES
153	e	1219.37	756.90704	YES	YES
154	e	1219.37	756.90677	YES	YES
155	e	1230.30	612.79532	YES	YES
156	e	1230.30	612.79568	YES	YES
157	b	1234.03	655.08511	YES	YES
158	a	1241.20	0.00000	NO	YES
159	e	1242.07	251.71110	YES	YES
160	e	1242.07	251.71081	YES	YES
161	a	1246.49	0.00000	NO	YES
162	b	1253.94	0.00000	YES	YES
163	b	1253.96	222.50119	YES	YES
164	a	1260.67	0.00000	NO	YES
165	e	1263.95	925.79401	YES	YES
166	e	1263.95	925.79422	YES	YES
167	b	1268.36	778.90369	YES	YES
168	b	1339.15	301.57597	YES	YES
169	e	1340.76	235.84951	YES	YES
170	e	1340.76	235.84948	YES	YES
171	a	1362.87	0.00000	NO	YES

$end

atom	charge
1 al	0.2185
2 f	-0.1655
3 f	-0.1827
4 f	-0.2002
5 f	-0.2013
6 f	-0.1865
7 f	-0.1588
8 f	-0.1444
9 f	-0.1942
10 f	-0.1743
11 o	-0.2438
12 c	0.5265
13 c	0.5405

```
 14 c   |    0.5385
 15 c   |   -0.0584
 16 f   |   -0.1655
 17 f   |   -0.1655
 18 f   |   -0.1655
 19 f   |   -0.1827
 20 f   |   -0.1827
 21 f   |   -0.1827
 22 f   |   -0.2002
 23 f   |   -0.2002
 24 f   |   -0.2002
 25 f   |   -0.2013
 26 f   |   -0.2013
 27 f   |   -0.2013
 28 f   |   -0.1865
 29 f   |   -0.1865
 30 f   |   -0.1865
 31 f   |   -0.1588
 32 f   |   -0.1588
 33 f   |   -0.1588
 34 f   |   -0.1444
 35 f   |   -0.1444
 36 f   |   -0.1444
 37 f   |   -0.1942
 38 f   |   -0.1942
 39 f   |   -0.1942
 40 f   |   -0.1743
 41 f   |   -0.1743
 42 f   |   -0.1743
 43 o   |   -0.2438
 44 o   |   -0.2438
 45 o   |   -0.2438
 46 c   |    0.5265
 47 c   |    0.5265
 48 c   |    0.5265
 49 c   |    0.5405
 50 c   |    0.5405
 51 c   |    0.5405
 52 c   |    0.5385
 53 c   |    0.5385
 54 c   |    0.5385
 55 c   |   -0.0584
 56 c   |   -0.0584
 57 c   |   -0.0584
-------------------------
```

$[Al(OC_5F_4N)_4]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Al   -0.2911083    0.2081726    0.1623243
F    -1.7236084   -3.9689433   -0.5257807
N     0.9851516   -4.9829641    1.6470946
C    -0.0270933   -2.6155000    0.4705972
O    -0.5032963   -1.5332120   -0.0956108
F    -0.6654336   -6.2068130    0.6667844
N     5.0335831    0.6304306   -1.8991997
C    -0.6374424   -3.8803028    0.2545937
O     1.2678187    0.9484057   -0.2008424
F     2.6572751   -3.8059692    2.6520582
N    -1.2172954    2.7845134   -4.6089108
C    -0.0841662   -5.0107283    0.8684571
O    -1.4871461    1.0807328   -0.8357035
F     1.7295432   -1.4404068    1.5638070
N    -3.8807825    0.8135191    4.3942643
C     1.5693876   -3.8164489    1.8638575
```

```
O    -0.6081165    0.6746835    1.8505633
F     2.1874058   -1.5067657   -1.2800417
C     1.1131508   -2.6150221    1.3155782
C     2.4468570    0.8136000   -0.7490425
F     4.7035354   -1.5787503   -2.3435981
C     2.9485551   -0.3988350   -1.2940859
F     5.4051761    2.8386982   -1.4770320
C     4.2362360   -0.4226484   -1.8418674
F     2.9135404    3.1209673   -0.3593924
F     0.2453982    0.0385815   -2.7625757
C     4.5844002    1.7748193   -1.4101536
C     3.3193487    1.9344774   -0.8348516
F     0.3629436    1.2622771   -5.2261579
C    -2.0470380    3.2602247   -3.6946930
F    -2.7525423    2.2232281    5.7820573
C    -0.4733664    1.7390268   -4.2893364
F    -0.5435471    2.1849770    4.1597931
C    -0.5207574    1.1134694   -3.0404276
F    -3.0415253    3.2597332   -1.5217256
C    -1.3924682    1.6091119   -2.0337324
F    -2.7941293    4.3247203   -4.0374775
C    -1.6357371    1.4765578    3.8394112
C    -1.6533092    0.7081849    2.6424079
F    -2.9416945   -0.7510728    1.2706337
C    -2.1856888    2.7283767   -2.4069378
F    -5.0528469   -0.5884879    3.0325615
C    -3.9209456    0.0895429    3.2884704
C    -2.7721487    1.4859524    4.6569774
C    -2.8560727   -0.0041137    2.3868851

SCF energy GEOOPT =  -3120.295240819 H
ZPE =   521.3 kJ/mol
FREEH energy =   627.22 kJ/mol
FREEH entropy =   1.08267 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   169.   169 a     -0.13956784 H =     -3.79783 eV
   LUMO:   170.   170 a     +0.02091297 H =     +0.56907 eV
   Gap :                    +0.16048082 H =     +4.36691 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)      km/mol          IR     RAMAN
     1                      -0.00        0.00000        -       -
     2                       0.00        0.00000        -       -
     3                       0.00        0.00000        -       -
     4                       0.00        0.00000        -       -
     5                       0.00        0.00000        -       -
     6                       0.00        0.00000        -       -
     7        a              5.25        0.07576       YES     YES
     8        a              6.80        0.05871       YES     YES
     9        a             12.97        0.07300       YES     YES
    10        a             14.66        0.06052       YES     YES
    11        a             19.80        0.02782       YES     YES
    12        a             24.26        0.03350       YES     YES
    13        a             24.99        0.10227       YES     YES
    14        a             29.78        0.01379       YES     YES
    15        a             35.54        0.05466       YES     YES
    16        a             50.99        0.11852       YES     YES
    17        a             57.48        0.09999       YES     YES
    18        a             68.63        0.29158       YES     YES
    19        a             83.20        1.76637       YES     YES
    20        a             94.16        1.50252       YES     YES
    21        a             95.01        1.96079       YES     YES
    22        a             98.48        1.18315       YES     YES
    23        a            100.31        0.62976       YES     YES
    24        a            117.52        0.03709       YES     YES
    25        a            118.88        0.08593       YES     YES
    26        a            122.38        0.21252       YES     YES
    27        a            127.70        0.24130       YES     YES
```

28	a	136.28	0.29845	YES	YES
29	a	165.04	0.48459	YES	YES
30	a	179.31	4.31203	YES	YES
31	a	187.94	0.68171	YES	YES
32	a	196.36	1.05975	YES	YES
33	a	211.50	2.58854	YES	YES
34	a	213.91	3.40522	YES	YES
35	a	222.68	1.11317	YES	YES
36	a	237.29	8.18884	YES	YES
37	a	263.43	15.15266	YES	YES
38	a	264.77	12.38933	YES	YES
39	a	267.32	9.51167	YES	YES
40	a	274.68	0.22984	YES	YES
41	a	276.37	2.55524	YES	YES
42	a	293.48	3.17947	YES	YES
43	a	294.93	1.57327	YES	YES
44	a	295.23	0.37283	YES	YES
45	a	310.28	1.53902	YES	YES
46	a	319.78	22.08871	YES	YES
47	a	326.95	28.47216	YES	YES
48	a	337.01	1.10888	YES	YES
49	a	337.57	2.49458	YES	YES
50	a	340.36	3.87941	YES	YES
51	a	343.85	19.73306	YES	YES
52	a	347.30	4.40303	YES	YES
53	a	349.84	2.24590	YES	YES
54	a	362.88	16.65705	YES	YES
55	a	369.42	37.27474	YES	YES
56	a	409.55	7.82921	YES	YES
57	a	426.07	0.31969	YES	YES
58	a	427.63	0.43422	YES	YES
59	a	428.29	0.04701	YES	YES
60	a	429.45	0.21529	YES	YES
61	a	436.02	51.02848	YES	YES
62	a	440.28	16.97222	YES	YES
63	a	441.93	9.00857	YES	YES
64	a	450.92	4.47833	YES	YES
65	a	452.05	1.25915	YES	YES
66	a	458.16	10.76456	YES	YES
67	a	460.87	12.36289	YES	YES
68	a	507.44	0.50703	YES	YES
69	a	534.48	65.21710	YES	YES
70	a	545.01	48.67532	YES	YES
71	a	547.28	48.46909	YES	YES
72	a	611.71	0.32467	YES	YES
73	a	618.86	0.24277	YES	YES
74	a	619.32	0.80013	YES	YES
75	a	620.16	1.00392	YES	YES
76	a	623.93	2.63282	YES	YES
77	a	626.36	0.82871	YES	YES
78	a	626.93	2.82565	YES	YES
79	a	628.53	1.22898	YES	YES
80	a	629.46	1.69175	YES	YES
81	a	630.34	3.35518	YES	YES
82	a	632.29	3.59704	YES	YES
83	a	632.77	5.24308	YES	YES
84	a	663.73	1.08988	YES	YES
85	a	672.71	6.62654	YES	YES
86	a	672.98	5.60927	YES	YES
87	a	674.40	5.03658	YES	YES
88	a	700.06	1.54716	YES	YES
89	a	724.94	32.16232	YES	YES
90	a	726.01	20.31641	YES	YES
91	a	728.07	7.85367	YES	YES
92	a	736.05	0.59589	YES	YES
93	a	760.17	88.12128	YES	YES
94	a	763.77	111.78020	YES	YES
95	a	779.63	120.57734	YES	YES
96	a	969.84	96.24069	YES	YES
97	a	971.47	12.74183	YES	YES

98	a	973.93	261.57008	YES	YES
99	a	974.29	440.85634	YES	YES
100	a	1126.76	738.89895	YES	YES
101	a	1129.96	622.83435	YES	YES
102	a	1134.48	463.49007	YES	YES
103	a	1144.96	45.76659	YES	YES
104	a	1149.50	1.76652	YES	YES
105	a	1150.10	99.59499	YES	YES
106	a	1151.56	10.74816	YES	YES
107	a	1152.33	5.17280	YES	YES
108	a	1299.91	0.89470	YES	YES
109	a	1303.79	3.57557	YES	YES
110	a	1305.79	3.37460	YES	YES
111	a	1317.24	2.98565	YES	YES
112	a	1376.30	18.63007	YES	YES
113	a	1377.59	24.44034	YES	YES
114	a	1378.29	51.03787	YES	YES
115	a	1381.19	31.37704	YES	YES
116	a	1421.05	34.80525	YES	YES
117	a	1421.62	24.97792	YES	YES
118	a	1421.71	65.87333	YES	YES
119	a	1422.74	21.54270	YES	YES
120	a	1486.43	148.34153	YES	YES
121	a	1487.92	104.07541	YES	YES
122	a	1490.23	759.34602	YES	YES
123	a	1490.74	1083.42134	YES	YES
124	a	1553.08	673.41676	YES	YES
125	a	1557.27	618.77698	YES	YES
126	a	1565.80	640.87378	YES	YES
127	a	1588.23	152.36675	YES	YES
128	a	1605.02	3.16303	YES	YES
129	a	1605.75	15.42396	YES	YES
130	a	1605.93	15.33683	YES	YES
131	a	1608.32	17.77922	YES	YES
132	a	1625.70	400.95559	YES	YES
133	a	1626.54	347.71825	YES	YES
134	a	1627.91	255.23528	YES	YES
135	a	1643.14	59.71916	YES	YES

$end

atom	charge
1 al	0.3020
2 f	-0.1776
3 n	-0.2080
4 c	0.0833
5 o	-0.2248
6 f	-0.1849
7 n	-0.2084
8 c	0.1517
9 o	-0.1875
10 f	-0.1834
11 n	-0.2083
12 c	0.2184
13 o	-0.2103
14 f	-0.1490
15 n	-0.2083
16 c	0.2310
17 o	-0.2006
18 f	-0.1621
19 c	0.1082
20 c	0.0799
21 f	-0.1838
22 c	0.1185
23 f	-0.1864
24 c	0.2273
25 f	-0.1779

```
 26 f   |   -0.1488
 27 c   |    0.2186
 28 c   |    0.1449
 29 f   |   -0.1826
 30 c   |    0.2182
 31 f   |   -0.1857
 32 c   |    0.2309
 33 f   |   -0.1784
 34 c   |    0.1039
 35 f   |   -0.1793
 36 c   |    0.0859
 37 f   |   -0.1850
 38 c   |    0.1500
 39 c   |    0.0782
 40 f   |   -0.1473
 41 c   |    0.1491
 42 f   |   -0.1844
 43 c   |    0.2289
 44 c   |    0.2176
 45 c   |    0.1066
-------------------------
```

$[B(OC_5F_4N)_4]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
F    -0.7792883    3.6247476   -0.6248928
C    -0.6698686    2.0306843    1.1513903
N     0.3070652    4.1197078    2.7754260
O    -1.1441015    1.0444229    0.3892100
B    -0.1814800    0.1702333   -0.2908177
C    -0.4833828    3.3402226    0.6444586
N     4.7876194    0.3979338   -1.7087959
O     0.7346961    1.0361535   -1.0671984
F     0.1853026    5.5749136    1.0278057
F     0.4422607    2.7123041    4.5625916
C     0.0075591    4.3316455    1.5060336
N     0.1668316   -4.3550873    2.2589218
O     0.6984531   -0.5661718    0.6472473
F    -0.4973288    0.6162859    3.0741590
C     0.1378226    2.9053824    3.2666915
N    -4.7924888   -0.6507665   -2.5633211
O    -0.9170681   -0.8123032   -1.0884372
F     2.5426868    3.0319751   -0.6703275
C    -0.3409187    1.8238628    2.5140973
F     5.2099751    2.5643486   -1.1457208
C     2.0194337    0.7807939   -1.2653884
F     4.4190805   -1.7760989   -2.2762893
C     2.9629783    1.8258493   -1.0835071
F     1.7357794   -1.5181577   -1.8817408
C     4.3187325    1.5721933   -1.3221676
C     3.9271618   -0.5911934   -1.8767072
F     2.7890513   -2.2538354    0.9350055
C     2.5461051   -0.4697990   -1.6783454
F     2.3976162   -4.7508311    2.0133638
C     0.4642205   -1.7663160    1.1542760
F    -2.0651421   -4.0042084    2.5310082
C     1.3519799   -3.9165364    1.8691459
F    -2.5230111   -2.9931355   -1.0126270
C     1.5651572   -2.6481834    1.3196687
F    -1.8995826   -1.4986388    1.5015632
C    -0.8702429   -3.5484382    2.1184804
F    -5.0718825   -2.8464649   -2.0222960
C    -2.1501183   -0.6995719   -1.5526862
F    -1.9785831    1.5858760   -2.2593469
C    -0.7958332   -2.2538848    1.5858791
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F    -4.5537971    1.5377590   -3.1442740
C    -4.2844564   -1.7567217   -2.0454186
C    -2.9874482   -1.8463973   -1.5289251
C    -4.0264147    0.4253994   -2.6025505
C    -2.7051310    0.4700469   -2.1346419

SCF energy GEOOPT =  -2902.666147856 H
ZPE =   534.0 kJ/mol
FREEH energy =   634.84 kJ/mol
FREEH entropy =   1.01136 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   165.   165 a     -0.13389738 H =     -3.64353 eV
   LUMO:   166.   166 a     +0.01949698 H =     +0.53054 eV
   Gap :                    +0.15339436 H =     +4.17407 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             12.76         0.03395       YES     YES
     8        a             17.16         0.00321       YES     YES
     9        a             20.02         0.03879       YES     YES
    10        a             22.93         0.04084       YES     YES
    11        a             24.27         0.01230       YES     YES
    12        a             26.19         0.04284       YES     YES
    13        a             30.38         0.01710       YES     YES
    14        a             33.81         0.05284       YES     YES
    15        a             42.55         0.04578       YES     YES
    16        a             65.30         0.24446       YES     YES
    17        a             74.61         0.14560       YES     YES
    18        a             80.01         0.26988       YES     YES
    19        a            106.90         0.79352       YES     YES
    20        a            111.94         0.09917       YES     YES
    21        a            114.27         0.10244       YES     YES
    22        a            117.27         0.02406       YES     YES
    23        a            120.30         0.03929       YES     YES
    24        a            121.95         0.06885       YES     YES
    25        a            126.44         0.05409       YES     YES
    26        a            129.22         0.02518       YES     YES
    27        a            132.55         0.06673       YES     YES
    28        a            139.09         0.06770       YES     YES
    29        a            198.93         3.19678       YES     YES
    30        a            207.17         0.48618       YES     YES
    31        a            208.73         0.87691       YES     YES
    32        a            211.54         0.97952       YES     YES
    33        a            235.42         1.64247       YES     YES
    34        a            249.34         2.31110       YES     YES
    35        a            268.15         2.50180       YES     YES
    36        a            272.11         0.78742       YES     YES
    37        a            274.38         0.95818       YES     YES
    38        a            275.51         1.17710       YES     YES
    39        a            282.74         0.35481       YES     YES
    40        a            296.11         0.02060       YES     YES
    41        a            297.30         0.56893       YES     YES
    42        a            301.45         0.27019       YES     YES
    43        a            308.13         0.27969       YES     YES
    44        a            317.21         1.78932       YES     YES
    45        a            330.30         1.19413       YES     YES
    46        a            332.73         1.36848       YES     YES
    47        a            341.15         2.56357       YES     YES
    48        a            344.61         1.02702       YES     YES
    49        a            346.46         2.61389       YES     YES
    50        a            356.36         0.19982       YES     YES
    51        a            365.01         7.77671       YES     YES
```

52	a	383.25	0.59391	YES	YES
53	a	408.87	0.64299	YES	YES
54	a	414.71	1.23106	YES	YES
55	a	428.10	0.25782	YES	YES
56	a	429.24	0.67762	YES	YES
57	a	430.43	0.96794	YES	YES
58	a	430.77	0.60792	YES	YES
59	a	440.03	0.07767	YES	YES
60	a	444.50	0.42148	YES	YES
61	a	448.62	1.75089	YES	YES
62	a	449.55	0.43223	YES	YES
63	a	459.52	0.35354	YES	YES
64	a	483.68	1.74833	YES	YES
65	a	497.75	5.36928	YES	YES
66	a	504.44	0.99946	YES	YES
67	a	517.51	2.06559	YES	YES
68	a	538.73	0.77684	YES	YES
69	a	602.51	25.74586	YES	YES
70	a	604.48	25.07356	YES	YES
71	a	608.23	31.41998	YES	YES
72	a	623.86	6.18514	YES	YES
73	a	627.16	0.72948	YES	YES
74	a	627.34	1.10952	YES	YES
75	a	629.20	1.96963	YES	YES
76	a	629.85	0.84875	YES	YES
77	a	631.61	0.66994	YES	YES
78	a	634.37	0.31610	YES	YES
79	a	638.90	0.17635	YES	YES
80	a	641.80	4.03773	YES	YES
81	a	650.41	11.56486	YES	YES
82	a	661.13	8.26578	YES	YES
83	a	674.71	0.50908	YES	YES
84	a	678.99	1.27887	YES	YES
85	a	684.61	4.67079	YES	YES
86	a	686.33	6.09200	YES	YES
87	a	695.32	10.66453	YES	YES
88	a	724.64	0.59733	YES	YES
89	a	727.78	0.56429	YES	YES
90	a	736.37	2.42779	YES	YES
91	a	737.72	2.80422	YES	YES
92	a	774.29	1.10656	YES	YES
93	a	917.62	236.21837	YES	YES
94	a	957.25	43.58568	YES	YES
95	a	963.32	50.16924	YES	YES
96	a	971.29	233.11527	YES	YES
97	a	975.38	54.54503	YES	YES
98	a	999.47	726.69174	YES	YES
99	a	1011.69	623.93319	YES	YES
100	a	1107.22	649.46170	YES	YES
101	a	1115.67	731.25656	YES	YES
102	a	1123.49	1025.80421	YES	YES
103	a	1141.39	49.64683	YES	YES
104	a	1149.62	32.32425	YES	YES
105	a	1152.65	7.97573	YES	YES
106	a	1152.95	29.01518	YES	YES
107	a	1157.64	22.82929	YES	YES
108	a	1295.53	0.98752	YES	YES
109	a	1300.65	10.06539	YES	YES
110	a	1303.86	9.02035	YES	YES
111	a	1318.45	1.10729	YES	YES
112	a	1371.62	0.11113	YES	YES
113	a	1377.81	1.82464	YES	YES
114	a	1378.08	8.98625	YES	YES
115	a	1378.21	18.09526	YES	YES
116	a	1422.42	21.69243	YES	YES
117	a	1422.86	33.13580	YES	YES
118	a	1423.18	39.96209	YES	YES
119	a	1424.40	8.19696	YES	YES
120	a	1481.09	378.55426	YES	YES
121	a	1481.77	116.90113	YES	YES

122	a	1486.71	383.97099	YES	YES
123	a	1488.85	1115.55044	YES	YES
124	a	1520.55	410.01933	YES	YES
125	a	1530.24	663.19027	YES	YES
126	a	1535.42	520.03471	YES	YES
127	a	1554.74	59.30783	YES	YES
128	a	1608.64	1.00716	YES	YES
129	a	1608.86	14.97479	YES	YES
130	a	1609.55	9.93782	YES	YES
131	a	1610.94	4.16024	YES	YES
132	a	1621.97	120.26680	YES	YES
133	a	1625.10	181.37789	YES	YES
134	a	1626.77	301.04121	YES	YES
135	a	1635.72	32.79648	YES	YES

$end

atom	charge
1 f	-0.1598
2 c	0.0650
3 n	-0.1949
4 o	-0.1434
5 b	-0.1792
6 c	0.1746
7 n	-0.2052
8 o	-0.1011
9 f	-0.1839
10 f	-0.1860
11 c	0.2205
12 n	-0.2058
13 o	-0.1055
14 f	-0.1712
15 c	0.2185
16 n	-0.2056
17 o	-0.0885
18 f	-0.1787
19 c	0.1610
20 f	-0.1875
21 c	0.0646
22 f	-0.1845
23 c	0.1585
24 f	-0.1626
25 c	0.2169
26 c	0.2306
27 f	-0.1772
28 c	0.1374
29 f	-0.1871
30 c	0.0687
31 f	-0.1843
32 c	0.2177
33 f	-0.1749
34 c	0.1565
35 f	-0.1593
36 c	0.2308
37 f	-0.1868
38 c	0.0645
39 f	-0.1537
40 c	0.1341
41 f	-0.1859
42 c	0.2172
43 c	0.1590
44 c	0.2231
45 c	0.1333

$[Al(OTeF_5)_4]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: s4

Cartesian coordinates in Ångström:
Al   -0.0000000   -0.0000000    0.0000000
O    -1.2676184   -0.8045769   -0.9672411
O    -0.8045769    1.2676184    0.9672411
O     0.8045769   -1.2676184    0.9672411
Te   -2.5087354    0.0811086   -2.0934990
Te   -0.0811086   -2.5087354    2.0934990
Te    0.0811086    2.5087354    2.0934990
F    -1.7711720   -1.5689115    1.9865882
F    -0.9678124   -3.7676362    3.2530271
F     0.3594234   -1.5318706    3.6930961
F     1.5203805   -3.5476505    2.3107830
F    -0.6158394   -3.6634448    0.6465429
F    -3.6634448    0.6158394   -0.6465429
F    -3.5476505   -1.5203805   -2.3107830
F    -3.7676362    0.9678124   -3.2530271
F    -1.5318706   -0.3594234   -3.6930961
F    -1.5689115    1.7711720   -1.9865882
F     1.7711720    1.5689115    1.9865882
F    -0.3594234    1.5318706    3.6930961
F     0.9678124    3.7676362    3.2530271
F    -1.5203805    3.5476505    2.3107830
F     0.6158394    3.6634448    0.6465429
F     1.5318706    0.3594234   -3.6930961
F     1.5689115   -1.7711720   -1.9865882
Te    2.5087354   -0.0811086   -2.0934990
F     3.7676362   -0.9678124   -3.2530271
O     1.2676184    0.8045769   -0.9672411
F     3.5476505    1.5203805   -2.3107830
F     3.6634448   -0.6158394   -0.6465429

SCF energy GEOOPT =  -2571.168925924 H
ZPE =   161.9 kJ/mol
FREEH energy =   265.95 kJ/mol
FREEH entropy =   1.07522 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   125.    62 e     -0.22687037 H =     -6.17346 eV
   LUMO:   126.    33 a     -0.11904669 H =     -3.23943 eV
   Gap :                    +0.10782368 H =     +2.93403 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                      -0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        e              8.26         0.10482       YES     YES
     8        e              8.26         0.10482       YES     YES
     9        b             13.55         0.00000       YES     YES
    10        b             17.80         0.01500       YES     YES
    11        b             19.49         0.06635       YES     YES
    12        e             29.70         0.02603       YES     YES
    13        e             29.70         0.02603       YES     YES
    14        a             30.51         0.00000       NO      YES
    15        b             31.60         0.00399       YES     YES
    16        e             50.39         0.21426       YES     YES
    17        e             50.39         0.21426       YES     YES
    18        a             57.24         0.00000       NO      YES
    19        a             81.02         0.00000       NO      YES
    20        b             82.22         6.18073       YES     YES
```

21	b	84.23	0.79278	YES	YES
22	e	87.61	2.77055	YES	YES
23	e	87.61	2.77055	YES	YES
24	a	113.71	0.00000	NO	YES
25	e	160.15	5.92561	YES	YES
26	e	160.15	5.92561	YES	YES
27	b	163.93	6.36647	YES	YES
28	a	167.85	0.00000	NO	YES
29	e	168.90	0.20611	YES	YES
30	e	168.90	0.20611	YES	YES
31	b	175.89	6.11955	YES	YES
32	a	177.23	0.00000	NO	YES
33	e	182.10	4.26477	YES	YES
34	e	182.10	4.26477	YES	YES
35	b	185.68	1.07625	YES	YES
36	a	194.84	0.00000	NO	YES
37	e	247.20	0.41999	YES	YES
38	e	247.20	0.41999	YES	YES
39	a	248.27	0.00000	NO	YES
40	b	249.00	0.54595	YES	YES
41	e	258.47	23.18648	YES	YES
42	e	258.47	23.18648	YES	YES
43	b	264.52	97.30042	YES	YES
44	e	270.32	31.82298	YES	YES
45	e	270.32	31.82298	YES	YES
46	a	272.39	0.00000	NO	YES
47	b	273.83	2.17080	YES	YES
48	e	274.97	46.29092	YES	YES
49	e	274.97	46.29090	YES	YES
50	b	280.24	0.00000	YES	YES
51	b	280.36	0.70466	YES	YES
52	e	282.44	45.80323	YES	YES
53	e	282.44	45.80324	YES	YES
54	a	293.84	0.00000	NO	YES
55	b	297.54	171.20719	YES	YES
56	a	307.20	0.00000	NO	YES
57	e	310.23	48.61021	YES	YES
58	e	310.23	48.61020	YES	YES
59	b	359.25	16.59342	YES	YES
60	a	451.80	0.00000	NO	YES
61	b	536.53	25.14054	YES	YES
62	e	547.42	28.29523	YES	YES
63	e	547.42	28.29523	YES	YES
64	b	580.55	1.45008	YES	YES
65	b	580.58	0.00000	YES	YES
66	e	585.45	1.48327	YES	YES
67	e	585.45	1.48326	YES	YES
68	a	586.85	0.00000	NO	YES
69	b	588.19	0.09603	YES	YES
70	e	588.49	12.94511	YES	YES
71	e	588.49	12.94510	YES	YES
72	a	614.19	0.00000	NO	YES
73	b	621.37	91.61968	YES	YES
74	e	623.80	101.12538	YES	YES
75	e	623.80	101.12538	YES	YES
76	e	640.54	22.90180	YES	YES
77	e	640.54	22.90180	YES	YES
78	a	643.22	0.00000	NO	YES
79	b	645.32	66.39310	YES	YES
80	a	647.92	0.00000	NO	YES
81	e	650.92	217.80341	YES	YES
82	e	650.92	217.80342	YES	YES
83	b	651.29	137.11016	YES	YES
84	b	806.57	524.93676	YES	YES
85	a	811.65	0.00000	NO	YES
86	e	819.77	391.51655	YES	YES
87	e	819.77	391.51655	YES	YES

$end

atom	charge
1 al	0.2068
2 o	-0.4708
3 o	-0.4708
4 o	-0.4708
5 te	2.1481
6 te	2.1481
7 te	2.1481
8 f	-0.3838
9 f	-0.4043
10 f	-0.3965
11 f	-0.3986
12 f	-0.3958
13 f	-0.3958
14 f	-0.3986
15 f	-0.4043
16 f	-0.3965
17 f	-0.3838
18 f	-0.3838
19 f	-0.3965
20 f	-0.4043
21 f	-0.3986
22 f	-0.3958
23 f	-0.3965
24 f	-0.3838
25 te	2.1481
26 f	-0.4043
27 o	-0.4708
28 f	-0.3986
29 f	-0.3958

$[Ga(OTeF_5)_4]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: s4

Cartesian coordinates in Ångström:

Ga	0.0000000	0.0000000	0.0000000
O	1.4431611	0.5926375	1.0236325
O	-0.5926375	1.4431611	-1.0236325
O	0.5926375	-1.4431611	-1.0236325
Te	1.2651023	2.1663897	2.0819575
Te	2.1663897	-1.2651023	-2.0819575
Te	-2.1663897	1.2651023	-2.0819575
F	2.2291354	0.6612670	-1.8696407
F	3.7449008	-1.0919417	-3.1732165
F	1.1636341	-1.0532952	-3.7132968
F	2.2407856	-3.1609953	-2.3947139
F	3.3705487	-1.4779839	-0.5908622
F	1.4779839	3.3705487	0.5908622
F	3.1609953	2.2407856	2.3947139
F	1.0919417	3.7449008	3.1732165
F	1.0532952	1.1636341	3.7132968
F	-0.6612670	2.2291354	1.8696407
F	-2.2291354	-0.6612670	-1.8696407
F	-1.1636341	1.0532952	-3.7132968
F	-3.7449008	1.0919417	-3.1732165
F	-2.2407856	3.1609953	-2.3947139
F	-3.3705487	1.4779839	-0.5908622
F	-1.0532952	-1.1636341	3.7132968
F	0.6612670	-2.2291354	1.8696407
Te	-1.2651023	-2.1663897	2.0819575
F	-1.0919417	-3.7449008	3.1732165
O	-1.4431611	-0.5926375	1.0236325
F	-3.1609953	-2.2407856	2.3947139

```
F    -1.4779839   -3.3705487    0.5908622

SCF energy GEOOPT =  -4253.586983625 H
ZPE =   157.9 kJ/mol
FREEH energy =   263.06 kJ/mol
FREEH entropy =   1.06350 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   134.    66 e     -0.22380001 H =     -6.08991 eV
   LUMO:   135.    35 a     -0.12128331 H =     -3.30029 eV
   Gap :                    +0.10251670 H =     +2.78962 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        e             17.17         0.08709       YES     YES
     8        e             17.17         0.08709       YES     YES
     9        b             17.24         0.00000       YES     YES
    10        b             17.62         0.02058       YES     YES
    11        b             23.54         0.00148       YES     YES
    12        a             31.45         0.00000       NO      YES
    13        e             34.48         0.08880       YES     YES
    14        e             34.48         0.08880       YES     YES
    15        b             35.98         0.04940       YES     YES
    16        e             60.40         0.04213       YES     YES
    17        e             60.40         0.04213       YES     YES
    18        a             64.47         0.00000       NO      YES
    19        b             79.59         3.33253       YES     YES
    20        e             81.80         3.94564       YES     YES
    21        e             81.80         3.94564       YES     YES
    22        b             83.86         4.65611       YES     YES
    23        a             84.55         0.00000       NO      YES
    24        a            113.32         0.00000       NO      YES
    25        e            156.49         8.44749       YES     YES
    26        e            156.49         8.44749       YES     YES
    27        b            162.09         8.22178       YES     YES
    28        a            163.89         0.00000       NO      YES
    29        e            167.32         0.28394       YES     YES
    30        e            167.32         0.28394       YES     YES
    31        b            168.82        12.47289       YES     YES
    32        a            170.55         0.00000       NO      YES
    33        e            174.94         1.46044       YES     YES
    34        e            174.94         1.46044       YES     YES
    35        b            181.57         0.70686       YES     YES
    36        a            200.16         0.00000       NO      YES
    37        e            222.79         9.22659       YES     YES
    38        e            222.79         9.22660       YES     YES
    39        b            230.69        26.12397       YES     YES
    40        e            246.18         2.29377       YES     YES
    41        e            246.18         2.29377       YES     YES
    42        a            246.55         0.00000       NO      YES
    43        b            248.55         0.78210       YES     YES
    44        e            268.14        51.67695       YES     YES
    45        e            268.14        51.67695       YES     YES
    46        b            276.53         0.00000       YES     YES
    47        b            276.59         3.67478       YES     YES
    48        e            277.34        17.02685       YES     YES
    49        e            277.34        17.02685       YES     YES
    50        a            278.82         0.00000       NO      YES
    51        b            279.90         0.20980       YES     YES
    52        e            280.22        53.92959       YES     YES
    53        e            280.22        53.92960       YES     YES
    54        b            286.58       216.99521       YES     YES
    55        e            289.43        47.95500       YES     YES
```

56	e	289.43	47.95499	YES	YES
57	a	291.28	0.00000	NO	YES
58	a	299.50	0.00000	NO	YES
59	b	314.03	6.60115	YES	YES
60	a	466.84	0.00000	NO	YES
61	b	506.40	12.59417	YES	YES
62	e	510.03	52.60224	YES	YES
63	e	510.03	52.60224	YES	YES
64	b	577.05	4.04268	YES	YES
65	a	577.56	0.00000	NO	YES
66	e	581.56	7.35424	YES	YES
67	e	581.56	7.35424	YES	YES
68	e	584.80	2.96935	YES	YES
69	e	584.80	2.96935	YES	YES
70	a	586.76	0.00000	NO	YES
71	b	587.61	1.26240	YES	YES
72	a	614.18	0.00000	NO	YES
73	b	615.29	61.75943	YES	YES
74	e	615.47	71.66935	YES	YES
75	e	615.47	71.66936	YES	YES
76	e	638.96	21.85720	YES	YES
77	e	638.96	21.85719	YES	YES
78	a	640.09	0.00000	NO	YES
79	b	641.97	40.88171	YES	YES
80	e	646.68	221.04228	YES	YES
81	e	646.68	221.04228	YES	YES
82	a	647.33	0.00000	NO	YES
83	b	649.80	180.06692	YES	YES
84	b	724.75	424.06116	YES	YES
85	e	727.03	297.90666	YES	YES
86	e	727.03	297.90666	YES	YES
87	a	766.52	0.00000	NO	YES

$end

atom	charge
1 ga	0.1971
2 o	-0.4634
3 o	-0.4634
4 o	-0.4634
5 te	2.1427
6 te	2.1427
7 te	2.1427
8 f	-0.3826
9 f	-0.4030
10 f	-0.3975
11 f	-0.3991
12 f	-0.3964
13 f	-0.3964
14 f	-0.3991
15 f	-0.4030
16 f	-0.3975
17 f	-0.3826
18 f	-0.3826
19 f	-0.3975
20 f	-0.4030
21 f	-0.3991
22 f	-0.3964
23 f	-0.3975
24 f	-0.3826
25 te	2.1427
26 f	-0.4030
27 o	-0.4634
28 f	-0.3991
29 f	-0.3964

$[Al(OC_{10}F_{15})_4]^-$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

C	-1.04186	-1.44280	5.61856
C	-2.10287	-0.79837	4.67378
C	-0.22935	-2.52018	4.83753
F	-1.65123	-2.00567	6.69589
F	-0.21055	-0.49363	6.11077
C	-3.07176	-1.90428	4.15315
C	-1.20254	-3.62426	4.32201
C	-2.26330	-2.98441	3.37207
F	-4.02046	-1.36236	3.35412
F	-3.73242	-2.47702	5.19399
F	-1.81952	-4.23409	5.36853
F	-0.51445	-4.59453	3.67619
C	-1.37998	-0.13297	3.46005
F	-2.81619	0.13849	5.37062
C	0.49303	-1.85012	3.62334
F	0.69092	-3.08453	5.67939
C	-1.53217	-2.31948	2.16450
F	-3.11845	-3.95636	2.93028
C	-0.54062	-1.18558	2.63262
F	-0.57089	0.85571	3.91298
F	-2.30274	0.45859	2.66446
F	1.22994	-2.78286	2.97394
F	1.36546	-0.92288	4.08714
F	-2.44949	-1.80369	1.30772
F	-0.86083	-3.27390	1.47863
O	0.11564	-0.61464	1.61226
F	3.91310	1.10585	-0.98726
F	5.55864	1.61672	0.95071
F	3.30027	0.40090	1.48063
F	5.35596	3.47306	-1.12114
C	3.29372	2.28879	-0.75853
F	2.82586	2.72108	-1.95368
O	1.21624	1.22425	-0.26618
C	4.92249	2.79846	1.13276
C	4.34042	3.31611	-0.21724
C	2.71659	1.61440	1.62546
C	2.09870	2.08814	0.25240
F	5.85952	3.66387	1.60379
F	4.28614	2.18572	3.35234
C	3.76996	2.63423	2.16827
F	1.74432	1.47474	2.55542
C	3.64677	4.69281	0.01622
F	3.17091	5.18184	-1.15259
C	1.44822	3.50481	0.50037
F	0.92973	3.98669	-0.65393
F	4.55035	5.60418	0.46589
C	3.07617	4.01247	2.39832
C	2.48972	4.53137	1.05097
F	0.41692	3.39237	1.37529
F	3.96848	4.90815	2.89875
F	2.09668	3.90049	3.32522
F	1.89550	5.74743	1.25268
F	-1.75509	0.00507	-2.93076
F	-2.30900	1.95175	-4.51618
F	-0.93185	2.42591	-2.34402
F	-4.20066	-0.06860	-4.19916
C	-2.87875	0.25031	-2.21793
F	-3.30093	-0.93829	-1.72528
O	-1.66467	0.77211	-0.16564
C	-3.43840	2.16270	-3.80125
C	-3.95813	0.82319	-3.19092
C	-2.09995	2.61028	-1.67831
C	-2.56776	1.24896	-1.03527

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F         -4.35119        2.66259       -4.67626
F         -2.72953        4.36599       -3.19604
C         -3.16972        3.18821       -2.65718
F         -1.85628        3.52106       -0.70586
C         -5.27843        1.08538       -2.40740
F         -5.76201       -0.07428       -1.90311
C         -3.92942        1.52625       -0.28735
F         -4.39941        0.38269        0.26603
F         -6.23769        1.56120       -3.24593
C         -4.49522        3.44431       -1.87505
C         -5.00959        2.10638       -1.26002
F         -3.73647        2.40068        0.72956
F         -5.43363        3.97008       -2.70742
F         -4.30052        4.36475       -0.90205
F         -6.17530        2.34222       -0.58196
F          0.47578       -1.00158       -3.98584
F          0.50895       -3.30520       -5.17798
F         -0.99934       -2.98701       -3.08646
F          2.87580       -1.84413       -5.06876
C          1.46573       -1.42507       -3.16317
F          2.19131       -0.32860       -2.83793
O          0.04977       -1.23160       -1.20619
C          1.51748       -3.67507       -4.35317
C          2.36847       -2.43317       -3.94260
C          0.04297       -3.35140       -2.30046
C          0.85874       -2.07723       -1.85677
F          2.27968       -4.55120       -5.06020
F          0.21224       -5.46050       -3.44435
C          0.94448       -4.36452       -3.07646
F         -0.48920       -3.96756       -1.21802
C          3.54518       -2.89037       -3.02770
F          4.31314       -1.83020       -2.68610
C          2.06854       -2.57533       -0.97436
F          2.81235       -1.51301       -0.57563
F          4.35748       -3.74719       -3.70234
C          2.12524       -4.82032       -2.16335
C          2.97688       -3.58046       -1.74901
F          1.60983       -3.16773        0.15282
F          2.90083       -5.72453       -2.81902
F          1.65199       -5.45574       -1.06548
F          4.01616       -3.98695       -0.95785
Al        -0.06556        0.05167       -0.00828

SCF energy GEOOPT =  -8053.020604483 H
ZPE =   1155. kJ/mol
FREEH energy =  1389.24 kJ/mol
FREEH entropy =   1.84778 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   413.   413 a     -0.16645056 H =     -4.52935 eV
   LUMO:   414.   414 a     +0.00792713 H =     +0.21571 eV
   Gap :                    +0.17437769 H =     +4.74506 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a               5.30         0.00857       YES     YES
     8        a              13.18         0.00849       YES     YES
     9        a              15.28         0.00649       YES     YES
    10        a              17.55         0.00585       YES     YES
    11        a              18.06         0.01841       YES     YES
    12        a              21.42         0.01732       YES     YES
    13        a              23.50         0.01168       YES     YES
    14        a              25.49         0.08732       YES     YES
```

15	a	26.71	0.05698	YES	YES
16	a	29.41	0.02276	YES	YES
17	a	43.51	0.09529	YES	YES
18	a	48.99	0.01086	YES	YES
19	a	54.45	0.00734	YES	YES
20	a	56.22	0.12313	YES	YES
21	a	64.14	0.81890	YES	YES
22	a	67.73	0.72480	YES	YES
23	a	67.94	0.68305	YES	YES
24	a	87.42	0.00176	YES	YES
25	a	131.91	0.01770	YES	YES
26	a	132.81	0.03412	YES	YES
27	a	133.85	0.02652	YES	YES
28	a	134.35	0.01910	YES	YES
29	a	135.34	0.00904	YES	YES
30	a	136.65	0.04992	YES	YES
31	a	138.83	0.04518	YES	YES
32	a	139.70	0.04930	YES	YES
33	a	141.07	0.47522	YES	YES
34	a	142.47	0.46468	YES	YES
35	a	144.23	0.70979	YES	YES
36	a	145.45	0.00613	YES	YES
37	a	193.58	0.54402	YES	YES
38	a	194.17	0.58533	YES	YES
39	a	194.99	0.40028	YES	YES
40	a	195.14	0.25057	YES	YES
41	a	195.68	0.44444	YES	YES
42	a	196.67	0.20435	YES	YES
43	a	197.32	0.12337	YES	YES
44	a	198.20	0.22555	YES	YES
45	a	198.89	0.14128	YES	YES
46	a	199.46	0.00898	YES	YES
47	a	200.29	0.40895	YES	YES
48	a	201.49	0.05353	YES	YES
49	a	202.53	0.01813	YES	YES
50	a	202.86	0.11361	YES	YES
51	a	203.08	0.08513	YES	YES
52	a	204.76	0.08131	YES	YES
53	a	205.02	0.05583	YES	YES
54	a	205.83	0.06592	YES	YES
55	a	206.16	0.05557	YES	YES
56	a	207.97	0.01457	YES	YES
57	a	224.55	0.01272	YES	YES
58	a	225.68	0.00245	YES	YES
59	a	225.98	0.00701	YES	YES
60	a	226.26	0.00620	YES	YES
61	a	242.01	0.28829	YES	YES
62	a	242.43	0.11890	YES	YES
63	a	243.03	0.47879	YES	YES
64	a	243.32	0.06885	YES	YES
65	a	243.82	0.19411	YES	YES
66	a	244.40	0.65296	YES	YES
67	a	244.68	0.47117	YES	YES
68	a	244.99	0.79458	YES	YES
69	a	245.28	0.07984	YES	YES
70	a	245.34	0.13137	YES	YES
71	a	245.55	0.23401	YES	YES
72	a	245.93	0.00339	YES	YES
73	a	246.02	0.11936	YES	YES
74	a	246.32	0.17186	YES	YES
75	a	246.42	0.35390	YES	YES
76	a	246.70	0.09506	YES	YES
77	a	247.11	0.01604	YES	YES
78	a	247.25	0.08933	YES	YES
79	a	247.35	0.13230	YES	YES
80	a	247.79	0.02719	YES	YES
81	a	251.65	2.95341	YES	YES
82	a	251.88	3.03135	YES	YES
83	a	253.14	2.72476	YES	YES
84	a	254.09	1.60029	YES	YES

85	a	255.25	0.74959	YES	YES
86	a	255.95	0.78458	YES	YES
87	a	256.78	0.12548	YES	YES
88	a	257.74	0.86187	YES	YES
89	a	258.53	0.32575	YES	YES
90	a	259.56	0.45898	YES	YES
91	a	260.06	0.27802	YES	YES
92	a	260.78	0.29679	YES	YES
93	a	262.56	0.01345	YES	YES
94	a	263.22	0.14721	YES	YES
95	a	263.44	0.15116	YES	YES
96	a	264.06	0.10876	YES	YES
97	a	268.36	0.40989	YES	YES
98	a	271.07	0.72710	YES	YES
99	a	273.52	5.42001	YES	YES
100	a	278.56	16.21236	YES	YES
101	a	281.48	19.91309	YES	YES
102	a	288.59	1.05850	YES	YES
103	a	293.84	11.28564	YES	YES
104	a	294.32	1.87011	YES	YES
105	a	296.25	3.82410	YES	YES
106	a	296.34	3.75326	YES	YES
107	a	296.79	13.89412	YES	YES
108	a	297.04	3.35519	YES	YES
109	a	297.53	1.64189	YES	YES
110	a	297.69	3.00446	YES	YES
111	a	297.90	0.44900	YES	YES
112	a	298.20	5.86066	YES	YES
113	a	298.40	6.57921	YES	YES
114	a	299.23	4.69267	YES	YES
115	a	299.66	9.24323	YES	YES
116	a	301.08	1.60563	YES	YES
117	a	301.50	2.23178	YES	YES
118	a	302.94	8.69576	YES	YES
119	a	306.12	0.19355	YES	YES
120	a	311.15	1.92554	YES	YES
121	a	312.22	2.87202	YES	YES
122	a	314.86	1.07872	YES	YES
123	a	330.78	6.08500	YES	YES
124	a	342.00	22.60759	YES	YES
125	a	361.73	1.21651	YES	YES
126	a	361.97	0.36482	YES	YES
127	a	363.35	1.15521	YES	YES
128	a	364.03	1.10519	YES	YES
129	a	373.08	23.03263	YES	YES
130	a	375.46	0.17202	YES	YES
131	a	376.26	0.17986	YES	YES
132	a	376.62	0.22927	YES	YES
133	a	377.06	0.58550	YES	YES
134	a	377.10	3.36361	YES	YES
135	a	377.43	2.91402	YES	YES
136	a	377.51	1.51204	YES	YES
137	a	378.00	0.27657	YES	YES
138	a	378.27	1.58486	YES	YES
139	a	378.41	0.45084	YES	YES
140	a	378.79	4.47651	YES	YES
141	a	380.06	0.03873	YES	YES
142	a	380.60	1.82742	YES	YES
143	a	380.98	3.34687	YES	YES
144	a	385.97	0.84952	YES	YES
145	a	386.67	1.15321	YES	YES
146	a	387.04	1.00241	YES	YES
147	a	388.11	0.84759	YES	YES
148	a	389.84	32.72750	YES	YES
149	a	391.15	7.77285	YES	YES
150	a	395.76	31.87443	YES	YES
151	a	399.56	45.55188	YES	YES
152	a	428.79	1.17770	YES	YES
153	a	429.88	5.51217	YES	YES
154	a	430.23	6.42144	YES	YES

155	a	430.30	12.20889	YES	YES
156	a	431.54	4.79153	YES	YES
157	a	432.05	0.18597	YES	YES
158	a	432.69	0.93237	YES	YES
159	a	432.73	14.38009	YES	YES
160	a	433.70	29.70940	YES	YES
161	a	434.03	28.25813	YES	YES
162	a	435.26	6.71077	YES	YES
163	a	436.19	43.20621	YES	YES
164	a	491.17	0.13446	YES	YES
165	a	522.69	13.23790	YES	YES
166	a	524.42	19.33356	YES	YES
167	a	526.58	22.74444	YES	YES
168	a	587.68	0.13683	YES	YES
169	a	588.43	0.11431	YES	YES
170	a	589.36	0.01905	YES	YES
171	a	589.72	0.01650	YES	YES
172	a	589.81	0.10057	YES	YES
173	a	590.00	0.04854	YES	YES
174	a	590.14	0.00476	YES	YES
175	a	590.48	0.16119	YES	YES
176	a	613.39	0.10751	YES	YES
177	a	628.04	19.78546	YES	YES
178	a	628.61	8.49965	YES	YES
179	a	629.09	15.77919	YES	YES
180	a	634.64	2.17967	YES	YES
181	a	634.90	15.12259	YES	YES
182	a	635.05	2.75888	YES	YES
183	a	635.35	5.88339	YES	YES
184	a	635.61	9.37901	YES	YES
185	a	635.67	9.22558	YES	YES
186	a	635.99	21.49282	YES	YES
187	a	636.04	21.77032	YES	YES
188	a	649.94	0.00802	YES	YES
189	a	666.32	18.03496	YES	YES
190	a	666.81	18.15553	YES	YES
191	a	667.78	18.61114	YES	YES
192	a	709.31	0.07833	YES	YES
193	a	754.79	21.11263	YES	YES
194	a	755.92	25.94393	YES	YES
195	a	761.40	25.41891	YES	YES
196	a	833.49	0.03849	YES	YES
197	a	833.61	0.02610	YES	YES
198	a	833.78	0.02746	YES	YES
199	a	833.89	0.09249	YES	YES
200	a	834.29	0.03550	YES	YES
201	a	834.65	0.01445	YES	YES
202	a	835.31	0.01334	YES	YES
203	a	835.67	0.01761	YES	YES
204	a	836.39	0.25387	YES	YES
205	a	836.54	0.34630	YES	YES
206	a	837.27	0.17420	YES	YES
207	a	837.91	0.48901	YES	YES
208	a	952.08	12.62124	YES	YES
209	a	952.25	22.38682	YES	YES
210	a	954.59	0.32556	YES	YES
211	a	957.28	25.32788	YES	YES
212	a	958.99	120.87394	YES	YES
213	a	960.06	677.03663	YES	YES
214	a	960.98	604.18892	YES	YES
215	a	961.76	622.85108	YES	YES
216	a	971.42	483.50705	YES	YES
217	a	972.50	557.44559	YES	YES
218	a	973.00	455.73474	YES	YES
219	a	978.48	10.31846	YES	YES
220	a	980.09	17.67636	YES	YES
221	a	980.98	11.90079	YES	YES
222	a	981.22	19.62927	YES	YES
223	a	982.39	26.05817	YES	YES
224	a	983.60	11.39895	YES	YES

225	a	983.98	16.40703	YES	YES
226	a	984.25	7.59072	YES	YES
227	a	985.01	9.36707	YES	YES
228	a	1023.97	3.13172	YES	YES
229	a	1025.66	1.56216	YES	YES
230	a	1026.40	5.90379	YES	YES
231	a	1027.29	1.46824	YES	YES
232	a	1028.45	3.02654	YES	YES
233	a	1028.98	3.68622	YES	YES
234	a	1029.24	3.93898	YES	YES
235	a	1029.64	0.93637	YES	YES
236	a	1054.34	1.04649	YES	YES
237	a	1054.70	0.61039	YES	YES
238	a	1054.83	1.03624	YES	YES
239	a	1055.20	1.70961	YES	YES
240	a	1055.25	1.05000	YES	YES
241	a	1055.86	1.16852	YES	YES
242	a	1056.55	1.56171	YES	YES
243	a	1056.78	1.28915	YES	YES
244	a	1065.49	0.14238	YES	YES
245	a	1066.80	0.49174	YES	YES
246	a	1067.53	0.90970	YES	YES
247	a	1068.72	1.39689	YES	YES
248	a	1093.89	75.07778	YES	YES
249	a	1094.15	75.59647	YES	YES
250	a	1095.83	66.20348	YES	YES
251	a	1098.43	11.90116	YES	YES
252	a	1118.08	0.54222	YES	YES
253	a	1120.09	0.23967	YES	YES
254	a	1120.62	1.32921	YES	YES
255	a	1121.01	1.53059	YES	YES
256	a	1121.29	0.30981	YES	YES
257	a	1121.83	0.07471	YES	YES
258	a	1122.46	1.30074	YES	YES
259	a	1122.95	0.86454	YES	YES
260	a	1127.73	0.37708	YES	YES
261	a	1129.73	0.03036	YES	YES
262	a	1130.77	0.19507	YES	YES
263	a	1131.38	0.39070	YES	YES
264	a	1196.74	1.19235	YES	YES
265	a	1197.23	0.98608	YES	YES
266	a	1197.95	1.28703	YES	YES
267	a	1199.47	1.22875	YES	YES
268	a	1199.63	0.81908	YES	YES
269	a	1201.02	1.25699	YES	YES
270	a	1204.11	6.45103	YES	YES
271	a	1204.89	7.51398	YES	YES
272	a	1205.33	4.75641	YES	YES
273	a	1205.98	14.85737	YES	YES
274	a	1206.85	7.41428	YES	YES
275	a	1207.44	12.84919	YES	YES
276	a	1208.15	8.70215	YES	YES
277	a	1208.73	17.83247	YES	YES
278	a	1209.61	11.93751	YES	YES
279	a	1209.94	8.88545	YES	YES
280	a	1210.97	5.58837	YES	YES
281	a	1211.30	1.96317	YES	YES
282	a	1212.07	5.85669	YES	YES
283	a	1212.38	6.43084	YES	YES
284	a	1232.18	22.01544	YES	YES
285	a	1233.00	28.32506	YES	YES
286	a	1233.67	13.76259	YES	YES
287	a	1235.27	0.71646	YES	YES
288	a	1244.47	13.82120	YES	YES
289	a	1246.62	7.09867	YES	YES
290	a	1248.52	947.33431	YES	YES
291	a	1248.90	929.10158	YES	YES
292	a	1250.27	897.88754	YES	YES
293	a	1252.02	143.60806	YES	YES
294	a	1252.99	9.89387	YES	YES

295	a	1253.19	77.82361	YES	YES
296	a	1254.12	50.46925	YES	YES
297	a	1254.47	17.67420	YES	YES
298	a	1255.01	20.21579	YES	YES
299	a	1255.41	86.92773	YES	YES
300	a	1255.68	40.51590	YES	YES
301	a	1256.60	90.05856	YES	YES
302	a	1256.85	117.87336	YES	YES
303	a	1257.40	245.84351	YES	YES
304	a	1259.91	518.37604	YES	YES
305	a	1261.46	542.76806	YES	YES
306	a	1261.51	47.20083	YES	YES
307	a	1263.13	315.83141	YES	YES
308	a	1280.08	146.22366	YES	YES
309	a	1280.59	159.79486	YES	YES
310	a	1280.95	166.05942	YES	YES
311	a	1288.76	0.91626	YES	YES
312	a	1361.67	438.38318	YES	YES
313	a	1363.43	468.03061	YES	YES
314	a	1368.14	457.02983	YES	YES
315	a	1398.84	13.78319	YES	YES

$end

atom	charge
1 c	0.4749
2 c	0.1846
3 c	0.1832
4 f	-0.2401
5 f	-0.2282
6 c	0.4739
7 c	0.4756
8 c	0.1866
9 f	-0.2247
10 f	-0.2404
11 f	-0.2403
12 f	-0.2273
13 c	0.4486
14 f	-0.2209
15 c	0.4686
16 f	-0.2224
17 c	0.4317
18 f	-0.2194
19 c	0.0448
20 f	-0.2267
21 f	-0.2129
22 f	-0.2281
23 f	-0.2280
24 f	-0.2081
25 f	-0.2150
26 o	-0.2885
27 f	-0.2258
28 f	-0.2277
29 f	-0.2192
30 f	-0.2224
31 c	0.4669
32 f	-0.2292
33 o	-0.2845
34 c	0.4747
35 c	0.1826
36 c	0.4351
37 c	0.0486
38 f	-0.2407
39 f	-0.2188
40 c	0.1840
41 f	-0.2059
42 c	0.4756

43	f	-0.2278
44	c	0.4486
45	f	-0.2222
46	f	-0.2404
47	c	0.4753
48	c	0.1842
49	f	-0.2214
50	f	-0.2407
51	f	-0.2256
52	f	-0.2211
53	f	-0.2059
54	f	-0.2248
55	f	-0.2142
56	f	-0.2194
57	c	0.4377
58	f	-0.2213
59	o	-0.2821
60	c	0.4752
61	c	0.1846
62	c	0.4437
63	c	0.0484
64	f	-0.2407
65	f	-0.2203
66	c	0.1854
67	f	-0.2213
68	c	0.4749
69	f	-0.2282
70	c	0.4693
71	f	-0.2278
72	f	-0.2408
73	c	0.4756
74	c	0.1825
75	f	-0.2296
76	f	-0.2407
77	f	-0.2280
78	f	-0.2229
79	f	-0.2270
80	f	-0.2282
81	f	-0.2291
82	f	-0.2210
83	c	0.4511
84	f	-0.2168
85	o	-0.2855
86	c	0.4749
87	c	0.1835
88	c	0.4662
89	c	0.0447
90	f	-0.2398
91	f	-0.2219
92	c	0.1833
93	f	-0.2267
94	c	0.4745
95	f	-0.2242
96	c	0.4268
97	f	-0.2082
98	f	-0.2402
99	c	0.4752
100	c	0.1875
101	f	-0.2116
102	f	-0.2401
103	f	-0.2271
104	f	-0.2196
105	al	0.1860

$[Ga(C_2F_5)_4]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Ga   -0.1799356   -0.0120167    0.2015486
F     0.2458433    1.8975687   -1.8692252
F     1.4207160    0.0388369   -2.1773604
F     1.9893023    2.5126701    0.2757506
F     2.8705139    2.3432005   -1.7150180
F     3.1643553    0.7494014   -0.2554455
C     0.9882155    0.9305617   -1.2056285
C     2.2662858    1.6423235   -0.7194280
F     1.9419896   -0.3977556    2.0703560
F     0.1333842   -1.5892922    2.5553575
F     2.3984369   -2.1040681   -0.1063765
F     2.4042344   -3.0248997    1.8743320
F     0.7035498   -3.3231687    0.5391113
C     0.9274187   -1.1556768    1.5037079
C     1.6147193   -2.4166142    0.9501360
F    -2.2610699    0.6321841    2.0222145
F    -0.3480757    1.6338703    2.5354371
F    -2.5111529    2.3936377   -0.1513845
F    -2.4211717    3.2977515    1.8336158
F    -0.6895875    3.4050209    0.5103306
C    -1.1634168    1.2772048    1.4706691
C    -1.7024787    2.6062745    0.9090143
F    -2.0212600   -2.1774761    0.1359202
F    -2.8054547   -0.3648229   -0.8767330
C    -1.6610059   -1.1286149   -0.6977398
F    -2.4145227   -2.5607063   -2.4783351
C    -1.3893254   -1.7646306   -2.0730876
F    -0.2760195   -2.5286547   -2.0468387
F    -1.2244882   -0.8121091   -3.0149005

SCF energy GEOOPT =  -4225.129207516 H
ZPE =   264.5 kJ/mol
FREEH energy =   344.32 kJ/mol
FREEH entropy =   0.84508 kJ/mol/K

HOMO-LUMO Separation
   HOMO:   130.   130 a     -0.11293347 H =     -3.07308 eV
   LUMO:   131.   131 a     +0.11788717 H =     +3.20787 eV
   Gap :                    +0.23082064 H =     +6.28095 eV

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             27.85         0.06330       YES     YES
     8        a             31.49         0.02004       YES     YES
     9        a             38.64         0.07547       YES     YES
    10        a             43.14         0.00275       YES     YES
    11        a             46.96         0.03723       YES     YES
    12        a             50.67         0.08596       YES     YES
    13        a             52.58         0.01991       YES     YES
    14        a             55.44         0.04020       YES     YES
    15        a             65.88         0.11748       YES     YES
    16        a             68.36         0.18713       YES     YES
    17        a             75.48         0.25613       YES     YES
    18        a             82.08         0.29040       YES     YES
    19        a             82.87         0.47595       YES     YES
    20        a             99.29         0.23747       YES     YES
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21	a	106.57	1.25620	YES	YES
22	a	111.57	0.47152	YES	YES
23	a	124.38	2.25934	YES	YES
24	a	173.33	0.23413	YES	YES
25	a	184.23	0.27536	YES	YES
26	a	197.96	1.04334	YES	YES
27	a	202.51	1.17428	YES	YES
28	a	210.94	0.36634	YES	YES
29	a	215.02	0.08767	YES	YES
30	a	217.15	0.61050	YES	YES
31	a	220.29	0.24861	YES	YES
32	a	221.79	0.13537	YES	YES
33	a	254.79	13.14368	YES	YES
34	a	264.62	2.19433	YES	YES
35	a	265.74	1.82239	YES	YES
36	a	273.74	1.95488	YES	YES
37	a	291.92	23.01648	YES	YES
38	a	301.32	31.05266	YES	YES
39	a	309.75	30.89396	YES	YES
40	a	354.09	0.44019	YES	YES
41	a	356.28	0.90881	YES	YES
42	a	356.33	0.11741	YES	YES
43	a	357.48	3.03734	YES	YES
44	a	413.27	0.02084	YES	YES
45	a	419.12	0.47655	YES	YES
46	a	419.74	0.50441	YES	YES
47	a	421.95	0.23596	YES	YES
48	a	516.12	2.07503	YES	YES
49	a	517.39	0.41156	YES	YES
50	a	517.57	0.65299	YES	YES
51	a	518.77	0.26076	YES	YES
52	a	567.69	1.38250	YES	YES
53	a	569.25	4.18228	YES	YES
54	a	570.08	2.05513	YES	YES
55	a	571.63	2.60899	YES	YES
56	a	581.16	2.25078	YES	YES
57	a	582.24	1.68683	YES	YES
58	a	588.45	3.23488	YES	YES
59	a	588.89	0.13273	YES	YES
60	a	715.74	27.83431	YES	YES
61	a	716.75	9.06849	YES	YES
62	a	717.00	1.90958	YES	YES
63	a	717.93	21.18781	YES	YES
64	a	912.13	38.10907	YES	YES
65	a	912.59	113.85323	YES	YES
66	a	921.53	115.85006	YES	YES
67	a	926.31	7.47195	YES	YES
68	a	1005.78	3.05605	YES	YES
69	a	1017.56	139.73927	YES	YES
70	a	1021.84	68.37955	YES	YES
71	a	1028.48	144.15251	YES	YES
72	a	1078.08	8.21624	YES	YES
73	a	1083.10	120.45885	YES	YES
74	a	1084.07	41.42974	YES	YES
75	a	1094.94	223.35963	YES	YES
76	a	1153.41	324.93767	YES	YES
77	a	1158.07	339.99172	YES	YES
78	a	1161.86	84.56219	YES	YES
79	a	1168.10	390.54194	YES	YES
80	a	1172.11	28.91006	YES	YES
81	a	1188.57	419.45153	YES	YES
82	a	1197.96	246.49760	YES	YES
83	a	1202.10	78.53938	YES	YES
84	a	1268.09	439.72871	YES	YES
85	a	1274.71	233.82380	YES	YES
86	a	1277.41	100.24267	YES	YES
87	a	1295.61	33.57510	YES	YES

$end

atom	charge
1 ga	-0.2178
2 f	-0.1914
3 f	-0.1926
4 f	-0.1748
5 f	-0.1966
6 f	-0.1758
7 c	0.2145
8 c	0.5175
9 f	-0.1880
10 f	-0.1897
11 f	-0.1775
12 f	-0.1966
13 f	-0.1770
14 c	0.2198
15 c	0.5161
16 f	-0.1894
17 f	-0.1898
18 f	-0.1753
19 f	-0.1981
20 f	-0.1788
21 c	0.2239
22 c	0.5165
23 f	-0.1868
24 f	-0.1907
25 c	0.2134
26 f	-0.1973
27 c	0.5161
28 f	-0.1771
29 f	-0.1769

AlF_3

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: cs

Cartesian coordinates in Ångström:
Al    0.0013727    0.0000000    0.0000000
F     1.6586727   -0.0000022    0.0000000
F    -0.8300245   -1.4337194    0.0000000
F    -0.8300209    1.4337216    0.0000000

SCF energy GEOOPT =  -541.8921547778 H
ZPE =   20.04 kJ/mol
FREEH energy =    31.87 kJ/mol
FREEH entropy =   0.29439 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a'           231.21        31.64752       YES     YES
     8        a'           231.52        32.52670       YES     YES
     9        a"           281.10       120.47193       YES     YES
    10        a'           680.48         0.00007       YES     YES
    11        a'           960.73       133.79773       YES     YES
    12        a'           964.84       134.60360       YES     YES
$end


Method: MP2/def-TZVPP
```

```
Symmetry: c2v

Cartesian coordinates in Ångström:
Al    0.0000000    0.0000000    0.0000001
F     0.0000000    0.0000000    1.6448484
F    -1.4244817    0.0000000   -0.8224243
F     1.4244817    0.0000000   -0.8224243

MP2 energy GEOOPT =  -541.4358886091 H
SCF energy GEOOPT =  -540.6103152235 H
ZPE =   20.72 kJ/mol
FREEH energy =    32.03 kJ/mol
FREEH entropy =   0.28443 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        b1           276.31        40.77174       YES     YES
     8        a1           276.31        40.77171       YES     YES
     9        b2           347.82       182.49115       YES     YES
    10        a1           685.44         0.00000       YES     YES
    11        b1           939.23       232.61777       YES     YES
    12        a1           939.24       232.62331       YES     YES
$end
```

$F_3Al\text{-}C_6F_5$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C    -1.8578237    0.5298491   -0.3410278
C    -0.5389089    1.0138994   -0.2646720
C     0.5676907    0.2024994    0.0113969
C    -2.0915218   -0.8361055   -0.1170510
C     0.2863050   -1.1527292    0.2180993
C    -1.0134066   -1.6909637    0.1599310
F    -2.8996861    1.3429725   -0.6195529
F    -0.3783719    2.3365101   -0.4990916
F     1.2781151   -2.0358608    0.4707333
F    -3.3457525   -1.3268834   -0.1818508
F    -1.2467714   -3.0054334    0.3665837
Al    2.4446636    0.9971724    0.1632779
F     2.2961024    2.5279539    0.8965612
F     3.3919746   -0.0267346    1.1402207
F     3.1073914    1.1238538   -1.4035580

SCF energy GEOOPT =  -1269.338730338 H
ZPE =   144.5 kJ/mol
FREEH energy =   182.96 kJ/mol
FREEH entropy =   0.51322 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                      -0.00         0.00000        -       -
     6                      -0.00         0.00000        -       -
     7        a             41.20         0.10914       YES     YES
```

```
     8        a              49.30         0.48315       YES     YES
     9        a              82.62         0.36870       YES     YES
    10        a             118.04         0.00675       YES     YES
    11        a             135.27         0.05848       YES     YES
    12        a             150.59         0.21358       YES     YES
    13        a             155.33         0.17812       YES     YES
    14        a             170.32         9.22652       YES     YES
    15        a             207.78         1.87239       YES     YES
    16        a             261.71         2.95721       YES     YES
    17        a             262.58         5.80703       YES     YES
    18        a             265.90         7.39173       YES     YES
    19        a             266.29         7.65888       YES     YES
    20        a             303.76         0.01482       YES     YES
    21        a             328.78        29.85213       YES     YES
    22        a             356.00         8.51712       YES     YES
    23        a             378.55        95.84781       YES     YES
    24        a             394.74         0.00935       YES     YES
    25        a             432.21         0.00599       YES     YES
    26        a             434.78         2.17360       YES     YES
    27        a             478.95        13.25759       YES     YES
    28        a             561.66         0.10817       YES     YES
    29        a             580.38         3.45181       YES     YES
    30        a             629.20         0.02493       YES     YES
    31        a             666.16       138.90788       YES     YES
    32        a             726.84         1.35576       YES     YES
    33        a             775.75         4.61682       YES     YES
    34        a             824.68       120.63054       YES     YES
    35        a             827.31        95.22993       YES     YES
    36        a             960.51       194.60179       YES     YES
    37        a            1065.43       232.12740       YES     YES
    38        a            1121.98         0.18270       YES     YES
    39        a            1242.91        33.56370       YES     YES
    40        a            1359.15         1.51088       YES     YES
    41        a            1361.32         3.91732       YES     YES
    42        a            1452.28       493.77425       YES     YES
    43        a            1497.87       118.43989       YES     YES
    44        a            1612.01        50.29229       YES     YES
    45        a            1615.43         1.87683       YES     YES
$end


Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
C    -1.8091894    0.4992756   -0.4418326
C    -0.5021397    0.9602832   -0.3350662
C     0.5714355    0.1725059    0.0544779
C    -2.0743456   -0.8293221   -0.1439354
C     0.2498153   -1.1458791    0.3399881
C    -1.0391174   -1.6633002    0.2509096
F    -2.8150443    1.3027271   -0.8237183
F    -0.3076287    2.2582066   -0.6373749
F     1.2001926   -2.0152252    0.7292492
F    -3.3248212   -1.3046891   -0.2372984
F    -1.3037523   -2.9486677    0.5376274
Al    2.4341205    1.0104833    0.1590998
F     2.3478060    2.2770213    1.2851019
F     3.5608125   -0.1523035    0.6573073
F     2.8118563    1.5788838   -1.3945355

MP2 energy GEOOPT =  -1268.3371821893 H
SCF energy GEOOPT =  -1265.360381547 H
ZPE =   157.6 kJ/mol
FREEH energy =   191.93 kJ/mol
FREEH entropy =   0.47482 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
```

```
#                      cm**(-1)        km/mol         IR     RAMAN
     1                    -0.00         0.00000        -       -
     2                    -0.00         0.00000        -       -
     3                    -0.00         0.00000        -       -
     4                    -0.00         0.00000        -       -
     5                    -0.00         0.00000        -       -
     6                     0.00         0.00000        -       -
     7        a           78.51         0.00092       YES     YES
     8        a           90.47         0.69937       YES     YES
     9        a          109.14         0.61284       YES     YES
    10        a          165.23         0.00081       YES     YES
    11        a          168.88         0.00286       YES     YES
    12        a          175.73         0.68243       YES     YES
    13        a          186.70         8.33627       YES     YES
    14        a          208.34         0.21983       YES     YES
    15        a          273.23        16.79562       YES     YES
    16        a          288.93        18.95378       YES     YES
    17        a          302.77         3.05524       YES     YES
    18        a          314.36         0.05919       YES     YES
    19        a          315.94         0.16471       YES     YES
    20        a          345.80         0.22184       YES     YES
    21        a          368.24        47.20780       YES     YES
    22        a          414.23       118.52021       YES     YES
    23        a          438.73         6.40393       YES     YES
    24        a          478.19         0.12541       YES     YES
    25        a          489.34         0.00491       YES     YES
    26        a          520.21         7.54462       YES     YES
    27        a          602.06         1.50774       YES     YES
    28        a          661.68       200.81059       YES     YES
    29        a          716.40         0.00174       YES     YES
    30        a          778.99         0.61977       YES     YES
    31        a          782.72       128.81582       YES     YES
    32        a          790.12       198.14245       YES     YES
    33        a          812.66        30.26078       YES     YES
    34        a          829.74         0.45081       YES     YES
    35        a          854.36         8.91678       YES     YES
    36        a         1007.32       280.37743       YES     YES
    37        a         1103.05         3.27186       YES     YES
    38        a         1114.17       266.77957       YES     YES
    39        a         1160.87         1.49949       YES     YES
    40        a         1331.73        56.20475       YES     YES
    41        a         1438.75         4.24888       YES     YES
    42        a         1543.90       541.97405       YES     YES
    43        a         1593.68       132.86647       YES     YES
    44        a         1740.08         0.67320       YES     YES
    45        a         1747.58        59.05327       YES     YES
$end
```

$F_3Al\text{-}OCH(CF_3)_2$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Al    2.3245867   -0.5345754    0.0783311
O     0.8511183    0.3933632   -0.3868372
C    -0.3872769   -0.0315839    0.0075134
C    -1.3027446   -0.2096697   -1.2227006
F    -0.7630160   -1.1088590   -2.0751332
F    -1.4923789    0.9390680   -1.9131132
F    -2.5398475   -0.6783677   -0.8838973
C    -0.9873051    0.9518450    1.0374374
F    -0.1755617    1.0428079    2.1135701
F    -2.2074188    0.5442895    1.4950218
F    -1.1479751    2.2012920    0.5428934
H    -0.3775142   -1.0267537    0.5225747
F     3.3311570    0.4280137    1.0543195
F     1.7082526   -1.8804357    0.9451306
```

```
F     3.1659243   -1.0304342   -1.3151104

SCF energy GEOOPT =  -1330.734268535 H
ZPE =   153.2 kJ/mol
FREEH energy =   190.84 kJ/mol
FREEH entropy =   0.51938 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             25.90         0.00516       YES     YES
     8        a             39.47         0.24153       YES     YES
     9        a             50.20         0.07739       YES     YES
    10        a             59.84         0.51407       YES     YES
    11        a            106.14         2.49258       YES     YES
    12        a            146.38         0.14966       YES     YES
    13        a            153.86         0.07935       YES     YES
    14        a            190.83         5.75187       YES     YES
    15        a            200.65         2.98316       YES     YES
    16        a            239.34         1.31271       YES     YES
    17        a            274.28        14.78628       YES     YES
    18        a            285.60         0.65638       YES     YES
    19        a            287.65        14.39508       YES     YES
    20        a            318.25        17.62211       YES     YES
    21        a            336.88        40.32356       YES     YES
    22        a            360.27        12.71539       YES     YES
    23        a            425.23        29.76155       YES     YES
    24        a            507.10         7.91394       YES     YES
    25        a            516.50         3.75147       YES     YES
    26        a            531.23         0.49045       YES     YES
    27        a            541.47        12.23358       YES     YES
    28        a            639.69        28.30717       YES     YES
    29        a            666.77        39.56308       YES     YES
    30        a            705.86         9.58642       YES     YES
    31        a            760.51        84.92902       YES     YES
    32        a            819.32       160.26474       YES     YES
    33        a            830.78       111.05511       YES     YES
    34        a            848.95        98.41975       YES     YES
    35        a            873.60        48.80078       YES     YES
    36        a           1084.60       110.59589       YES     YES
    37        a           1115.98        74.56914       YES     YES
    38        a           1159.35       405.40411       YES     YES
    39        a           1202.96       141.40322       YES     YES
    40        a           1213.23       461.03506       YES     YES
    41        a           1239.58       159.07778       YES     YES
    42        a           1272.89       147.26769       YES     YES
    43        a           1330.46         5.34106       YES     YES
    44        a           1363.95        62.37228       YES     YES
    45        a           2894.98        29.02314       YES     YES
$end


Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
Al    2.3268838   -0.5482530    0.0470294
O     0.8398792    0.3863349   -0.2996425
C    -0.4072979   -0.0285142    0.0575969
C    -1.2667553   -0.2227543   -1.1937662
F    -0.7070740   -1.1450969   -1.9842838
F    -1.4056384    0.8944049   -1.9171981
F    -2.5092170   -0.6619294   -0.9025422
```

```
C    -1.0268368    0.9735017    1.0346082
F    -0.2628962    1.0650249    2.1285798
F    -2.2553770    0.5978638    1.4481068
F    -1.1448431    2.2047265    0.5237780
H    -0.4295273   -0.9937630    0.5782222
F     3.3639027    0.3637727    1.0272194
F     1.7753575   -1.9448104    0.8549593
F     3.1094400   -0.9405082   -1.4026672

MP2 energy GEOOPT =  -1329.8341509725 H
SCF energy GEOOPT =  -1326.806035198 H
ZPE =   167.7 kJ/mol
FREEH energy =   201.91 kJ/mol
FREEH entropy =   0.47587 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             69.19         0.45721       YES     YES
     8        a             77.63         0.00364       YES     YES
     9        a            123.20         0.00289       YES     YES
    10        a            126.87         2.35399       YES     YES
    11        a            139.25         1.63770       YES     YES
    12        a            170.77         0.02704       YES     YES
    13        a            174.40         0.45398       YES     YES
    14        a            227.79         8.81551       YES     YES
    15        a            229.34         3.15400       YES     YES
    16        a            271.70         6.51987       YES     YES
    17        a            299.04        17.39205       YES     YES
    18        a            327.82        14.83428       YES     YES
    19        a            331.10         0.33813       YES     YES
    20        a            353.21        28.73823       YES     YES
    21        a            379.11        43.35466       YES     YES
    22        a            407.10         9.81129       YES     YES
    23        a            461.22        40.53246       YES     YES
    24        a            562.36         6.69242       YES     YES
    25        a            571.44         4.73112       YES     YES
    26        a            583.09         6.12568       YES     YES
    27        a            588.57         0.46922       YES     YES
    28        a            657.08        94.56653       YES     YES
    29        a            731.26        35.72671       YES     YES
    30        a            744.32        49.49933       YES     YES
    31        a            786.30       152.65437       YES     YES
    32        a            793.27       201.76671       YES     YES
    33        a            805.67       123.97240       YES     YES
    34        a            924.60       134.19491       YES     YES
    35        a            936.11        97.11396       YES     YES
    36        a           1175.83       120.15991       YES     YES
    37        a           1198.50        93.17963       YES     YES
    38        a           1250.42       687.78949       YES     YES
    39        a           1264.33       151.36248       YES     YES
    40        a           1302.85       321.36561       YES     YES
    41        a           1387.04       141.13931       YES     YES
    42        a           1412.77       135.11864       YES     YES
    43        a           1532.29         0.29148       YES     YES
    44        a           1561.14        67.02793       YES     YES
    45        a           3098.44        17.32284       YES     YES
$end
```

$F_3Al\text{-}OC(CF_3)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
O    -0.6079574   -0.4454518    0.7808883
C     0.4118584   -0.0626107   -0.0020057
C     0.6377249    1.5032117    0.0516662
F    -0.2074825    2.1580880   -0.7681290
F     1.9016411    1.8570343   -0.3193583
F     0.4415283    1.9596170    1.2981163
C     1.7103886   -0.7771284    0.5369831
F     2.7505646   -0.7342813   -0.3368539
F     1.4618610   -2.0694487    0.8032546
F     2.1312803   -0.2015646    1.6874851
C     0.1782915   -0.4888969   -1.5006990
F    -1.0472409   -0.1248936   -1.9082380
F     0.2740054   -1.8300835   -1.6372739
F     1.0780867    0.0674819   -2.3567053
Al   -2.4003560   -0.2398949    0.8769437
F    -2.7902989   -0.6069455    2.4887964
F    -2.7813318    1.3716437    0.4951622
F    -3.1425634   -1.3358770   -0.1900328

SCF energy GEOOPT =  -1667.543223797 H
ZPE =   163.2 kJ/mol
FREEH energy =   210.33 kJ/mol
FREEH entropy =   0.58011 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             33.67         0.19263       YES     YES
     8        a             58.09         0.03014       YES     YES
     9        a             69.12         0.19297       YES     YES
    10        a             71.27         0.62167       YES     YES
    11        a             72.46         0.12647       YES     YES
    12        a             86.27         0.05869       YES     YES
    13        a            133.53         0.55513       YES     YES
    14        a            139.73         2.84491       YES     YES
    15        a            154.03         0.47036       YES     YES
    16        a            164.34         0.25730       YES     YES
    17        a            174.01         2.22892       YES     YES
    18        a            212.25         8.39425       YES     YES
    19        a            256.37         1.50438       YES     YES
    20        a            266.68         7.45175       YES     YES
    21        a            281.29         1.33760       YES     YES
    22        a            283.32        12.64687       YES     YES
    23        a            287.00        12.48411       YES     YES
    24        a            305.19         6.73986       YES     YES
    25        a            318.17         2.92644       YES     YES
    26        a            323.27         5.00455       YES     YES
    27        a            359.50        26.39833       YES     YES
    28        a            366.15        49.57054       YES     YES
    29        a            442.24        34.20821       YES     YES
    30        a            517.16         5.29010       YES     YES
    31        a            518.29         4.35214       YES     YES
    32        a            521.90         3.36761       YES     YES
    33        a            532.94        10.02724       YES     YES
    34        a            551.45         0.53584       YES     YES
    35        a            554.60         2.42700       YES     YES
    36        a            662.76        68.90218       YES     YES
```

```
    37        a             705.76        32.31728       YES     YES
    38        a             706.05        33.43782       YES     YES
    39        a             732.65        26.29536       YES     YES
    40        a             784.51        55.01383       YES     YES
    41        a             838.70       117.52978       YES     YES
    42        a             841.73       118.41630       YES     YES
    43        a             952.91       156.47186       YES     YES
    44        a             961.09       171.76217       YES     YES
    45        a            1106.76        15.31829       YES     YES
    46        a            1118.46         8.72985       YES     YES
    47        a            1123.80        14.78904       YES     YES
    48        a            1199.04        12.89976       YES     YES
    49        a            1204.96        13.44835       YES     YES
    50        a            1217.50       765.82918       YES     YES
    51        a            1236.24        29.11486       YES     YES
    52        a            1246.58       476.00725       YES     YES
    53        a            1252.99       484.74289       YES     YES
    54        a            1337.44       190.68463       YES     YES
$end


Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
O    -0.6206095   -0.4003554    0.7646456
C     0.4131382   -0.0450799   -0.0088289
C     0.6739117    1.4954224    0.0561198
F    -0.1626825    2.1624740   -0.7393843
F     1.9254180    1.8219288   -0.3205954
F     0.5020845    1.9449537    1.2949438
C     1.6767914   -0.7845533    0.5280906
F     2.7060653   -0.7656551   -0.3360878
F     1.4042465   -2.0585085    0.7912686
F     2.1034204   -0.2236583    1.6663296
C     0.1885654   -0.4501910   -1.4968573
F    -1.0297624   -0.1048717   -1.8951276
F     0.3067318   -1.7734826   -1.6525532
F     1.0697491    0.1289457   -2.3318655
Al   -2.4062800   -0.2597861    0.8774218
F    -2.7629987   -0.5263105    2.5088389
F    -2.8727870    1.2917092    0.3857410
F    -3.1150023   -1.4529813   -0.0920997

MP2 energy GEOOPT =  -1666.4725413789 H
SCF energy GEOOPT =  -1662.552825753 H
ZPE =   179.5 kJ/mol
FREEH energy =   222.03 kJ/mol
FREEH entropy =   0.53039 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                       -0.00         0.00000        -       -
     2                       -0.00         0.00000        -       -
     3                       -0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              74.53         0.24154       YES     YES
     8        a              85.67         0.03807       YES     YES
     9        a              92.85         0.85932       YES     YES
    10        a             141.13         0.99196       YES     YES
    11        a             146.55         0.04109       YES     YES
    12        a             149.56         0.12909       YES     YES
    13        a             164.38         1.76180       YES     YES
    14        a             167.93         1.73614       YES     YES
    15        a             175.73         1.21501       YES     YES
    16        a             199.12         0.23953       YES     YES
```

17	a	205.14	1.77909	YES	YES
18	a	252.52	9.73548	YES	YES
19	a	283.47	11.67665	YES	YES
20	a	291.08	15.81986	YES	YES
21	a	331.51	11.43160	YES	YES
22	a	331.65	1.73012	YES	YES
23	a	334.43	5.22868	YES	YES
24	a	343.05	13.79436	YES	YES
25	a	363.15	2.64861	YES	YES
26	a	367.97	9.78760	YES	YES
27	a	403.50	74.51507	YES	YES
28	a	411.85	12.93044	YES	YES
29	a	479.62	36.62864	YES	YES
30	a	569.29	1.27623	YES	YES
31	a	574.65	7.26270	YES	YES
32	a	576.62	9.68066	YES	YES
33	a	583.84	0.77995	YES	YES
34	a	610.46	0.76519	YES	YES
35	a	612.76	1.20276	YES	YES
36	a	668.36	144.18354	YES	YES
37	a	769.55	11.36721	YES	YES
38	a	770.18	19.32046	YES	YES
39	a	783.17	34.66703	YES	YES
40	a	796.82	199.38537	YES	YES
41	a	800.99	200.77091	YES	YES
42	a	824.60	31.40829	YES	YES
43	a	1033.29	276.01398	YES	YES
44	a	1042.19	289.74711	YES	YES
45	a	1196.15	12.81005	YES	YES
46	a	1214.45	45.21463	YES	YES
47	a	1219.67	42.27764	YES	YES
48	a	1302.99	1028.15731	YES	YES
49	a	1310.76	135.27218	YES	YES
50	a	1315.00	118.01376	YES	YES
51	a	1336.85	22.96098	YES	YES
52	a	1418.14	356.88193	YES	YES
53	a	1426.87	353.62640	YES	YES
54	a	1448.93	19.25432	YES	YES

$end

$F_3Al\text{-}OC_5F_4N$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Al    1.8891900   -0.3006525   -2.1452758
F     1.9897185   -1.9836720   -2.3299834
F     0.7401564    0.4373575   -3.1524365
N    -2.1182149    0.1872696    1.7613038
O     1.4240209    0.0766845   -0.4103844
F    -1.0713384    1.3644579    3.4096300
F     1.3020896    1.3326407    2.0444001
C     0.2127988    0.7378669    1.5230836
C     0.3067022    0.0943469    0.2487458
F    -0.9199575   -1.1751166   -1.3675226
F    -3.1988309   -0.9956266    0.1401891
C    -2.0602579   -0.4244432    0.5877958
C    -1.0045052    0.7468068    2.2089446
C    -0.9077563   -0.5143081   -0.1975026
F     3.4161847    0.4163882   -2.3209876

SCF energy GEOOPT =  -1261.452103165 H
ZPE =   149.3 kJ/mol
FREEH energy =   186.76 kJ/mol
FREEH entropy =   0.51592 kJ/mol/K

$vibrational spectrum
```

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.08	0.90729	YES	YES
8	a	51.31	0.08594	YES	YES
9	a	64.41	0.39865	YES	YES
10	a	111.16	0.61571	YES	YES
11	a	119.43	0.54505	YES	YES
12	a	146.66	2.44666	YES	YES
13	a	172.04	3.32393	YES	YES
14	a	186.99	2.80150	YES	YES
15	a	218.29	0.96183	YES	YES
16	a	250.03	14.18521	YES	YES
17	a	274.65	7.43551	YES	YES
18	a	294.11	6.77683	YES	YES
19	a	294.54	20.71854	YES	YES
20	a	333.28	41.27114	YES	YES
21	a	335.64	23.68673	YES	YES
22	a	358.75	31.73796	YES	YES
23	a	419.29	0.19811	YES	YES
24	a	432.14	23.39872	YES	YES
25	a	452.69	2.53125	YES	YES
26	a	515.76	30.18415	YES	YES
27	a	604.51	4.73461	YES	YES
28	a	615.59	1.05208	YES	YES
29	a	619.26	0.82279	YES	YES
30	a	642.22	8.77008	YES	YES
31	a	676.84	38.89847	YES	YES
32	a	717.16	98.31084	YES	YES
33	a	740.72	52.56153	YES	YES
34	a	842.93	119.53708	YES	YES
35	a	851.65	137.96763	YES	YES
36	a	966.57	223.18836	YES	YES
37	a	1127.55	341.57575	YES	YES
38	a	1134.85	0.81368	YES	YES
39	a	1308.43	8.14464	YES	YES
40	a	1366.74	75.86021	YES	YES
41	a	1408.24	29.05530	YES	YES
42	a	1484.16	485.68481	YES	YES
43	a	1576.92	388.51451	YES	YES
44	a	1592.42	8.07102	YES	YES
45	a	1629.11	305.38144	YES	YES

$end

Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

Al	1.5927779	-0.5025651	-2.3343368
F	1.5151340	-2.1862343	-2.2095428
F	0.4784054	0.1317593	-3.4352405
N	-1.8151604	0.2581496	2.0676290
O	1.2589780	0.2110672	-0.6991757
F	-0.5387536	1.5365116	3.4300968
F	1.5084137	1.5462369	1.6676045
C	0.3820479	0.8884741	1.3752142
C	0.2780719	0.2059757	0.1455060
F	-1.1664793	-1.1263608	-1.1768739
F	-3.0959783	-1.0189210	0.7108381
C	-1.9330715	-0.3848358	0.9261685
C	-0.6712544	0.8760483	2.2676212
C	-0.9550380	-0.4486511	-0.0483098
F	3.1619065	0.0133454	-2.6871988

```
MP2 energy GEOOPT =  -1260.4396106287 H
SCF energy GEOOPT =  -1257.440182757 H
ZPE =   161.7 kJ/mol
FREEH energy =   195.18 kJ/mol
FREEH entropy =   0.47019 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000         -       -
     2                      -0.00         0.00000         -       -
     3                       0.00         0.00000         -       -
     4                       0.00         0.00000         -       -
     5                       0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
     7        a             82.61         0.68743       YES     YES
     8        a             91.06         0.04318       YES     YES
     9        a             94.68         0.61029       YES     YES
    10        a            159.70         0.10716       YES     YES
    11        a            170.78         0.05273       YES     YES
    12        a            171.34         1.78480       YES     YES
    13        a            190.62         7.64168       YES     YES
    14        a            230.27         2.40834       YES     YES
    15        a            279.88        20.68651       YES     YES
    16        a            284.19         1.16549       YES     YES
    17        a            323.37        11.49663       YES     YES
    18        a            327.90        29.10588       YES     YES
    19        a            341.48         1.91362       YES     YES
    20        a            377.25        83.67537       YES     YES
    21        a            406.85        36.83202       YES     YES
    22        a            426.15         8.07071       YES     YES
    23        a            478.02        20.69540       YES     YES
    24        a            498.52         2.29131       YES     YES
    25        a            503.94         0.00006       YES     YES
    26        a            550.99        24.88434       YES     YES
    27        a            656.70       105.05850       YES     YES
    28        a            714.97       102.84384       YES     YES
    29        a            757.65        59.39229       YES     YES
    30        a            778.45         3.88681       YES     YES
    31        a            796.45         0.26766       YES     YES
    32        a            804.97       194.54484       YES     YES
    33        a            809.00       208.63997       YES     YES
    34        a            811.51         3.18525       YES     YES
    35        a            875.18        22.08233       YES     YES
    36        a           1019.98       288.33398       YES     YES
    37        a           1152.48        17.79207       YES     YES
    38        a           1186.86       127.88282       YES     YES
    39        a           1191.77       376.76597       YES     YES
    40        a           1381.53         8.16589       YES     YES
    41        a           1476.46         3.54743       YES     YES
    42        a           1565.83       623.41692       YES     YES
    43        a           1605.67       772.62522       YES     YES
    44        a           1716.95        14.64937       YES     YES
    45        a           1741.00       189.19621       YES     YES
$end
```

$F_3Al\text{-}OTeF_5$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Al    0.6289025   -1.6596836   -1.0765966
F     2.2846343   -1.4127615   -0.8292525
F     0.2686660   -2.0868630   -2.6767566
F    -0.0612635   -2.7153710    0.0500635
F     1.1350069    2.1416720    0.2135969
```

```
F     0.6251002   -0.0458960    1.7788827
Te   -0.4250905    1.0517934    0.5749382
F    -0.6673568    2.2202357    2.1020104
O    -0.2349171   -0.0195949   -0.9504624
F    -1.5088239    2.3342772   -0.3844133
F    -2.0448582    0.1921916    1.1979897

SCF energy GEOOPT =  -1124.173413894 H
ZPE =   60.11 kJ/mol
FREEH energy =    96.88 kJ/mol
FREEH entropy =   0.50788 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              28.75         0.07518       YES     YES
     8        a              51.52         0.24766       YES     YES
     9        a              68.02         0.54505       YES     YES
    10        a             123.84         2.23163       YES     YES
    11        a             128.47         0.45514       YES     YES
    12        a             154.53         1.50802       YES     YES
    13        a             174.87         2.52817       YES     YES
    14        a             176.64         1.00489       YES     YES
    15        a             198.38        16.35649       YES     YES
    16        a             243.45         0.17796       YES     YES
    17        a             256.28        21.30489       YES     YES
    18        a             259.84         0.63162       YES     YES
    19        a             281.99        24.95803       YES     YES
    20        a             287.02        34.39552       YES     YES
    21        a             287.52        83.61633       YES     YES
    22        a             312.02        51.89114       YES     YES
    23        a             344.29        22.60463       YES     YES
    24        a             486.64        64.00331       YES     YES
    25        a             571.49         1.66632       YES     YES
    26        a             576.01         0.22721       YES     YES
    27        a             599.49        48.20232       YES     YES
    28        a             632.92       113.64760       YES     YES
    29        a             634.62       116.78505       YES     YES
    30        a             684.30        63.08633       YES     YES
    31        a             771.53       197.94650       YES     YES
    32        a             854.40       112.16481       YES     YES
    33        a             860.18       130.84063       YES     YES
$end


Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
Al    0.6123400   -1.6493401   -1.0880128
F     2.2698883   -1.4592876   -0.8317846
F     0.2591701   -2.0048405   -2.6995789
F    -0.0692757   -2.7701769   -0.0258975
F     1.0589815    2.0982937    0.2144028
F     0.5863489    0.0706609    1.7921711
Te   -0.4206750    1.0643273    0.6060009
F    -0.6861714    2.2361410    2.0144616
O    -0.1918280   -0.0395575   -0.8045173
F    -1.4636675    2.2266956   -0.3791204
F    -1.9551113    0.2270841    1.2018751

MP2 energy GEOOPT =  -1123.4757037492 H
SCF energy GEOOPT =  -1120.966389047 H
```

```
ZPE =   69.51 kJ/mol
FREEH energy =   101.56 kJ/mol
FREEH entropy =   0.45811 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                       -0.00         0.00000        -       -
     2                       -0.00         0.00000        -       -
     3                       -0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              94.37         0.03597       YES     YES
     8        a             105.48         0.27710       YES     YES
     9        a             106.16         2.12405       YES     YES
    10        a             174.09         1.11354       YES     YES
    11        a             175.64         0.55181       YES     YES
    12        a             187.49         7.50407       YES     YES
    13        a             249.90         5.41519       YES     YES
    14        a             260.02         0.63785       YES     YES
    15        a             268.70        19.33116       YES     YES
    16        a             289.66        13.84189       YES     YES
    17        a             295.37         6.62600       YES     YES
    18        a             335.26         0.00457       YES     YES
    19        a             370.98       227.38350       YES     YES
    20        a             379.96        30.26552       YES     YES
    21        a             380.68        13.99599       YES     YES
    22        a             414.67        86.82417       YES     YES
    23        a             416.08         6.44641       YES     YES
    24        a             528.87        81.95471       YES     YES
    25        a             619.04         2.45026       YES     YES
    26        a             621.50         2.19043       YES     YES
    27        a             662.58       167.40568       YES     YES
    28        a             704.16        19.86724       YES     YES
    29        a             706.54       162.31654       YES     YES
    30        a             708.76       181.95200       YES     YES
    31        a             811.99       244.02203       YES     YES
    32        a             813.75       241.05125       YES     YES
    33        a             940.18       280.82120       YES     YES
$end
```

$F_3Al\text{-}OC_{10}F_{15}$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
F    -2.4510508   -3.5326002    0.7187401
F     1.3152894   -1.6032213   -1.6889698
F     2.8917436   -1.0332046    0.2985019
F     0.6652444   -2.3137774    0.7727001
F     2.6965086    0.8038516   -1.7878762
C     0.6520879   -0.4378853   -1.4759504
F     0.2096055   -0.0206128   -2.6890685
O    -1.3853493   -1.5767701   -1.0524621
C     2.2098350    0.1278990    0.4537514
C     1.6537517    0.6193371   -0.9157137
C     0.0279284   -1.1237128    0.8936606
C    -0.5717738   -0.6801622   -0.5040382
F     3.1100860    1.0246192    0.9447077
F     1.5382159   -0.4793108    2.6630737
C     1.0343974   -0.0644483    1.4574404
F    -0.9609682   -1.2960722    1.8025121
C     0.9131011    1.9752160   -0.7144695
F     0.4532515    2.4426460   -1.9000273
C    -1.2667655    0.7258611   -0.2731978
F    -1.7849201    1.1840671   -1.4401481
```

```
F     1.7801251    2.9197978   -0.2539571
C     0.3003376    1.2964456    1.6541742
C    -0.2646279    1.7882410    0.2879831
F    -2.3014084    0.6055505    0.5928844
F     1.1581140    2.2228131    2.1679795
F    -0.6948385    1.1707105    2.5629209
F    -0.8909379    2.9952675    0.4682858
F    -4.1596151   -1.5803195   -0.3699459
F    -3.0494169   -3.5627774   -2.0263879
Al   -2.8279506   -2.5974484   -0.6471031

SCF energy GEOOPT =  -2494.631303118 H
ZPE =   307.6 kJ/mol
FREEH energy =   377.05 kJ/mol
FREEH entropy =   0.71498 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                      -0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             21.87         0.55749       YES     YES
     8        a             38.85         0.49015       YES     YES
     9        a             59.37         0.65393       YES     YES
    10        a            117.70         3.28524       YES     YES
    11        a            118.89         0.20348       YES     YES
    12        a            134.02         0.00217       YES     YES
    13        a            147.70         0.06947       YES     YES
    14        a            149.73         0.01697       YES     YES
    15        a            156.66         5.49619       YES     YES
    16        a            194.87         0.30388       YES     YES
    17        a            196.97         0.22596       YES     YES
    18        a            201.92         0.61320       YES     YES
    19        a            203.78         0.43338       YES     YES
    20        a            204.62         0.64050       YES     YES
    21        a            225.36         0.00465       YES     YES
    22        a            242.30         0.92375       YES     YES
    23        a            243.80         0.44440       YES     YES
    24        a            244.57         0.71838       YES     YES
    25        a            244.86         0.72325       YES     YES
    26        a            246.49         0.08461       YES     YES
    27        a            251.07         2.29030       YES     YES
    28        a            252.61         2.86525       YES     YES
    29        a            258.29         5.11737       YES     YES
    30        a            259.69         4.95336       YES     YES
    31        a            261.34         5.32738       YES     YES
    32        a            263.60         0.36175       YES     YES
    33        a            292.60         5.78210       YES     YES
    34        a            295.54         1.08946       YES     YES
    35        a            296.11        15.67976       YES     YES
    36        a            296.84         5.17067       YES     YES
    37        a            298.50         7.62615       YES     YES
    38        a            323.04         9.68178       YES     YES
    39        a            336.34        82.20751       YES     YES
    40        a            361.41         0.41949       YES     YES
    41        a            373.43         0.02399       YES     YES
    42        a            374.70        10.21975       YES     YES
    43        a            375.11        18.50021       YES     YES
    44        a            377.59         1.08327       YES     YES
    45        a            385.81         4.73412       YES     YES
    46        a            390.77         8.89231       YES     YES
    47        a            429.25         8.85386       YES     YES
    48        a            430.68         9.37516       YES     YES
    49        a            433.91        10.84037       YES     YES
    50        a            508.25        14.29287       YES     YES
    51        a            587.47         0.01886       YES     YES
```

```
    52        a             588.75         0.05639       YES     YES
    53        a             607.82         8.99799       YES     YES
    54        a             633.33        13.52886       YES     YES
    55        a             633.98        13.05553       YES     YES
    56        a             642.01         1.20799       YES     YES
    57        a             676.94        58.46041       YES     YES
    58        a             727.81       100.19836       YES     YES
    59        a             830.26         7.32982       YES     YES
    60        a             834.61         0.03587       YES     YES
    61        a             835.49         0.57424       YES     YES
    62        a             841.62       103.67072       YES     YES
    63        a             842.75       112.13919       YES     YES
    64        a             951.36       254.32566       YES     YES
    65        a             957.33       296.48502       YES     YES
    66        a             968.11       313.39922       YES     YES
    67        a             972.08        49.40219       YES     YES
    68        a             977.60        29.85370       YES     YES
    69        a            1010.54         0.37473       YES     YES
    70        a            1016.41         0.93832       YES     YES
    71        a            1051.50         2.14319       YES     YES
    72        a            1053.72         1.81318       YES     YES
    73        a            1070.48         0.04094       YES     YES
    74        a            1083.63        27.98246       YES     YES
    75        a            1112.11         0.04182       YES     YES
    76        a            1116.90         0.37241       YES     YES
    77        a            1129.74         0.02572       YES     YES
    78        a            1197.93         3.34506       YES     YES
    79        a            1199.66         2.31789       YES     YES
    80        a            1204.47        15.11813       YES     YES
    81        a            1205.46         7.72862       YES     YES
    82        a            1207.79        13.74011       YES     YES
    83        a            1227.43         1.96249       YES     YES
    84        a            1244.95       403.56535       YES     YES
    85        a            1248.18        69.13558       YES     YES
    86        a            1250.88        89.16147       YES     YES
    87        a            1253.13       369.46382       YES     YES
    88        a            1256.72       375.68291       YES     YES
    89        a            1280.54        60.34938       YES     YES
    90        a            1374.21       281.86875       YES     YES
$end


Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
F    -2.1225410   -3.8132657    0.4462296
F     1.2742562   -1.6049898   -1.6535491
F     2.8257968   -1.0527652    0.3423179
F     0.5905743   -2.2701258    0.7797105
F     2.6993467    0.7419626   -1.7445190
C     0.6381691   -0.4360731   -1.4574702
F     0.2302250   -0.0253597   -2.6720164
O    -1.4295673   -1.5089918   -1.0563211
C     2.1671323    0.1096299    0.4758566
C     1.6465277    0.5950088   -0.8935456
C    -0.0246068   -1.0806830    0.8798020
C    -0.5882091   -0.6354690   -0.5091923
F     3.0697191    0.9826069    0.9704786
F     1.4501399   -0.4629273    2.6585121
C     0.9805767   -0.0472051    1.4505568
F    -1.0295759   -1.2414653    1.7577219
C     0.9450811    1.9584519   -0.7181012
F     0.5232766    2.4260967   -1.9045635
C    -1.2471634    0.7705742   -0.3091162
F    -1.7302254    1.2278715   -1.4797997
F     1.8173150    2.8785192   -0.2558167
C     0.2801016    1.3171389    1.6240461
C    -0.2418062    1.8050813    0.2557240
```

```
F    -2.2957775    0.6846646    0.5231440
F     1.1354601    2.2205234    2.1481564
F    -0.7273737    1.2197995    2.5048575
F    -0.8452369    3.0151338    0.4145005
F    -4.0146484   -1.7894732    0.1123513
F    -3.2250738   -3.3328463   -2.0803905
Al   -2.7518928   -2.6514229   -0.6095646

MP2 energy GEOOPT =  -2492.9831770076 H
SCF energy GEOOPT =  -2486.649259548 H
ZPE =   342.3 kJ/mol
FREEH energy =   404.30 kJ/mol
FREEH entropy =   0.64699 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             67.90         0.77285       YES     YES
     8        a             74.90         1.15417       YES     YES
     9        a             83.31         0.13459       YES     YES
    10        a            148.60         5.41207       YES     YES
    11        a            156.79         0.16915       YES     YES
    12        a            171.84         0.11223       YES     YES
    13        a            173.88         1.66137       YES     YES
    14        a            181.62         0.06764       YES     YES
    15        a            185.45         1.85459       YES     YES
    16        a            235.42         0.48347       YES     YES
    17        a            236.59         0.47595       YES     YES
    18        a            239.96         1.12502       YES     YES
    19        a            245.69         0.16761       YES     YES
    20        a            246.96         0.33168       YES     YES
    21        a            276.00         0.35836       YES     YES
    22        a            279.12         9.44474       YES     YES
    23        a            282.06        14.80952       YES     YES
    24        a            289.34         0.61996       YES     YES
    25        a            290.45         1.70370       YES     YES
    26        a            291.25         0.57171       YES     YES
    27        a            291.84         0.42619       YES     YES
    28        a            292.66         0.43021       YES     YES
    29        a            299.43         3.58603       YES     YES
    30        a            309.56         1.55164       YES     YES
    31        a            310.05         3.35656       YES     YES
    32        a            315.98         0.00439       YES     YES
    33        a            334.79         6.67119       YES     YES
    34        a            334.94         8.68316       YES     YES
    35        a            335.70        12.38406       YES     YES
    36        a            338.84         1.16509       YES     YES
    37        a            340.45         1.22786       YES     YES
    38        a            373.96         8.65361       YES     YES
    39        a            381.37       103.08239       YES     YES
    40        a            394.36         2.26187       YES     YES
    41        a            420.87        19.94617       YES     YES
    42        a            421.81         0.33663       YES     YES
    43        a            424.87         0.08461       YES     YES
    44        a            428.82         6.73491       YES     YES
    45        a            438.31         3.14360       YES     YES
    46        a            442.53         6.48916       YES     YES
    47        a            478.17        11.98330       YES     YES
    48        a            481.54        16.27554       YES     YES
    49        a            484.72        17.14348       YES     YES
    50        a            550.41        10.93210       YES     YES
    51        a            643.34        43.28754       YES     YES
    52        a            647.68         1.16526       YES     YES
    53        a            648.59         0.18385       YES     YES
```

54	a	683.80	43.20486	YES	YES
55	a	690.46	14.46608	YES	YES
56	a	690.80	11.64650	YES	YES
57	a	709.08	82.95351	YES	YES
58	a	759.41	43.25899	YES	YES
59	a	800.86	174.38433	YES	YES
60	a	808.16	193.65073	YES	YES
61	a	924.84	0.41960	YES	YES
62	a	928.77	0.00785	YES	YES
63	a	929.25	0.32330	YES	YES
64	a	1028.52	492.38032	YES	YES
65	a	1031.44	503.64597	YES	YES
66	a	1046.86	553.26273	YES	YES
67	a	1056.07	6.63493	YES	YES
68	a	1058.40	0.47488	YES	YES
69	a	1113.40	1.73168	YES	YES
70	a	1115.21	2.70822	YES	YES
71	a	1170.14	0.76581	YES	YES
72	a	1171.82	3.10655	YES	YES
73	a	1178.41	35.24335	YES	YES
74	a	1183.10	1.60234	YES	YES
75	a	1273.51	0.58003	YES	YES
76	a	1277.17	0.29341	YES	YES
77	a	1303.77	0.20702	YES	YES
78	a	1314.51	22.60925	YES	YES
79	a	1315.21	25.92956	YES	YES
80	a	1320.41	28.87620	YES	YES
81	a	1356.00	5.71610	YES	YES
82	a	1374.72	92.91951	YES	YES
83	a	1376.78	84.68932	YES	YES
84	a	1395.27	174.17330	YES	YES
85	a	1395.71	180.56582	YES	YES
86	a	1399.61	282.40192	YES	YES
87	a	1417.19	239.25713	YES	YES
88	a	1432.15	122.04818	YES	YES
89	a	1433.69	131.79085	YES	YES
90	a	1445.57	59.63181	YES	YES

$end

$F_3Al\text{-}C_2F_5$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

Al	-0.9495870	1.2041997	-0.6400437
F	1.3577071	0.7956152	1.0415750
F	-0.4727154	-0.2246654	1.8071176
F	1.6401540	-1.0843050	-0.8857619
F	1.4193977	-1.9672349	1.0967422
F	-0.2404644	-2.0473270	-0.3201895
C	0.2216615	0.0877486	0.6326580
C	0.7654588	-1.2579706	0.1311366
F	-0.1794657	1.2724154	-2.1602416
F	-2.4828922	0.4702909	-0.7679678
F	-1.0792543	2.7512331	0.0649751

SCF energy GEOOPT = -1117.033536944 H
ZPE = 85.47 kJ/mol
FREEH energy = 116.43 kJ/mol
FREEH entropy = 0.46022 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

```
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              31.23         0.19704      YES     YES
     8        a              59.66         0.07296      YES     YES
     9        a              79.12         1.24842      YES     YES
    10        a             107.02         0.48111      YES     YES
    11        a             149.61         0.03799      YES     YES
    12        a             192.14         2.83206      YES     YES
    13        a             200.10         9.91987      YES     YES
    14        a             214.74         0.36253      YES     YES
    15        a             248.92         9.37140      YES     YES
    16        a             276.64        14.45171      YES     YES
    17        a             285.36        10.62227      YES     YES
    18        a             353.55         0.79536      YES     YES
    19        a             384.10       105.06418      YES     YES
    20        a             418.47         0.04708      YES     YES
    21        a             514.51         1.60732      YES     YES
    22        a             567.03         1.36639      YES     YES
    23        a             578.63         2.49832      YES     YES
    24        a             668.45       114.96752      YES     YES
    25        a             717.03        12.38902      YES     YES
    26        a             822.25       102.32649      YES     YES
    27        a             825.16       114.11472      YES     YES
    28        a             915.73        29.64218      YES     YES
    29        a             986.29       132.91387      YES     YES
    30        a            1089.72       112.69675      YES     YES
    31        a            1147.82       263.75724      YES     YES
    32        a            1177.16       287.03019      YES     YES
    33        a            1279.34       140.39472      YES     YES
$end


Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
Al   -0.9324396    1.2282394   -0.6580309
F     1.4144506    0.7638749    0.9377321
F    -0.3971523   -0.1428725    1.8126938
F     1.4569953   -1.2025739   -0.9577858
F     1.4782832   -1.9089651    1.0825684
F    -0.3192571   -2.0916946   -0.0997701
C     0.2450798    0.0927179    0.6037989
C     0.7205108   -1.2872892    0.1580461
F    -0.0591480    1.5151106   -2.0820213
F    -2.3566325    0.3651892   -0.9734725
F    -1.2506902    2.6682633    0.1762413

MP2 energy GEOOPT =  -1116.2765358678 H
SCF energy GEOOPT =  -1113.888540562 H
ZPE =   93.08 kJ/mol
FREEH energy =   121.46 kJ/mol
FREEH entropy =   0.42879 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                       -0.00         0.00000        -       -
     2                       -0.00         0.00000        -       -
     3                       -0.00         0.00000        -       -
     4                       -0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              85.62         0.06411      YES     YES
     8        a             114.70         1.45586      YES     YES
     9        a             128.51         0.23909      YES     YES
    10        a             149.18         0.29494      YES     YES
    11        a             173.43         0.37465      YES     YES
```

```
    12        a             218.61         9.46276       YES     YES
    13        a             233.84         6.06680       YES     YES
    14        a             262.63         0.30436       YES     YES
    15        a             283.77        19.60177       YES     YES
    16        a             307.89        17.39111       YES     YES
    17        a             320.79         6.66967       YES     YES
    18        a             394.02         2.18270       YES     YES
    19        a             422.77       138.57909       YES     YES
    20        a             467.59         0.12126       YES     YES
    21        a             565.43         0.71861       YES     YES
    22        a             623.20         1.74388       YES     YES
    23        a             629.41         5.28197       YES     YES
    24        a             664.62       156.63698       YES     YES
    25        a             771.91         9.78864       YES     YES
    26        a             793.40       174.85531       YES     YES
    27        a             795.95       191.88361       YES     YES
    28        a             987.26        70.27638       YES     YES
    29        a            1039.12       187.42680       YES     YES
    30        a            1173.56       202.53678       YES     YES
    31        a            1248.21       229.82993       YES     YES
    32        a            1260.99       338.27077       YES     YES
    33        a            1445.81       131.72856       YES     YES
$end
```

$C_6F_5^-$

```
Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
F     0.1379973   -0.1494365    2.4733125
F     2.0674968    1.1787484    1.0995722
C     0.0628867   -0.0681041    1.1269783
C     1.0434534    0.6082985    0.4137399
F    -1.9407353   -1.3160174    1.1724736
C    -0.9952130   -0.6605399    0.4508234
C     0.9210075    0.6640336   -0.9724585
C    -1.0275353   -0.5486788   -0.9370122
F     1.9368505    1.3542672   -1.6009965
C    -0.0947958    0.1026528   -1.6990800
F    -2.1114127   -1.1652238   -1.5273527

MP2 energy GEOOPT =  -726.7812411061 H
SCF energy GEOOPT =  -724.6278322054 H
ZPE =   128.3 kJ/mol
FREEH energy =   148.93 kJ/mol
FREEH entropy =   0.36871 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a            155.34         0.00000       YES     YES
     8        a            200.67         0.32938       YES     YES
     9        a            272.96         0.17752       YES     YES
    10        a            310.76         0.99221       YES     YES
    11        a            314.16         0.00958       YES     YES
    12        a            339.67         0.10103       YES     YES
    13        a            369.29         0.00563       YES     YES
    14        a            380.50         8.55155       YES     YES
    15        a            474.60         0.64838       YES     YES
    16        a            488.85         0.95751       YES     YES
    17        a            505.56         0.00000       YES     YES
```

18	a	587.68	0.16573	YES	YES
19	a	644.42	8.53888	YES	YES
20	a	707.83	12.10214	YES	YES
21	a	769.15	10.20971	YES	YES
22	a	771.73	0.00000	YES	YES
23	a	833.39	0.77624	YES	YES
24	a	948.26	388.98046	YES	YES
25	a	1043.89	299.00274	YES	YES
26	a	1069.47	0.36150	YES	YES
27	a	1188.34	13.94202	YES	YES
28	a	1254.62	19.49895	YES	YES
29	a	1338.75	2.19288	YES	YES
30	a	1492.87	578.16300	YES	YES
31	a	1553.91	114.91694	YES	YES
32	a	1707.46	33.28962	YES	YES
33	a	1732.81	0.92817	YES	YES

$end

$CH(CF_3)_2O^-$

Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

O	-1.0742990	1.3111462	-0.7375415
C	-0.0494347	0.6147616	-0.3111999
C	0.0866818	-0.7481635	-1.0354645
F	1.1702403	-1.4882674	-0.6670872
F	-0.9795212	-1.5524172	-0.8807213
F	0.2269493	-0.5470247	-2.3601602
C	-0.0844359	0.3798695	1.2199328
F	-1.1675896	-0.2974013	1.6394186
F	-0.0998702	1.5642838	1.8614836
F	0.9921576	-0.2877708	1.7226386
H	0.9791215	1.0509838	-0.4512992

MP2 energy GEOOPT = -788.2551393291 H
SCF energy GEOOPT = -786.0490171972 H
ZPE = 135.8 kJ/mol
FREEH energy = 156.90 kJ/mol
FREEH entropy = 0.37197 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	120.06	0.00066	YES	YES
8	a	143.56	3.64301	YES	YES
9	a	201.09	0.86860	YES	YES
10	a	285.60	7.59282	YES	YES
11	a	294.25	9.87039	YES	YES
12	a	320.20	0.66987	YES	YES
13	a	347.29	1.30823	YES	YES
14	a	375.69	2.78278	YES	YES
15	a	494.22	0.27591	YES	YES
16	a	555.06	6.61787	YES	YES
17	a	560.77	5.93039	YES	YES
18	a	580.15	0.34968	YES	YES
19	a	634.31	2.08576	YES	YES
20	a	724.53	39.54099	YES	YES
21	a	766.97	7.38921	YES	YES
22	a	888.50	98.97842	YES	YES
23	a	898.69	101.80311	YES	YES

```
    24        a            1131.23          5.86727       YES     YES
    25        a            1146.79        226.60973       YES     YES
    26        a            1197.00        566.88930       YES     YES
    27        a            1259.71        310.43880       YES     YES
    28        a            1284.65        219.79264       YES     YES
    29        a            1364.42        177.20442       YES     YES
    30        a            1374.78        128.35698       YES     YES
    31        a            1483.97         14.52629       YES     YES
    32        a            1510.68         20.05603       YES     YES
    33        a            2764.60        234.94910       YES     YES
$end
```

$C(CF_3)_3O^-$

```
Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
O    -1.4140880   -0.2755796    1.1239813
C    -0.4091308   -0.0797361    0.3252011
C     0.0642862    1.4243248    0.3251069
F    -0.7974532    2.1991611   -0.3615159
F     1.2874886    1.6515964   -0.2149333
F     0.1068918    1.9110485    1.5684895
C     0.8440322   -0.9496865    0.7240416
F     1.8071187   -1.0560410   -0.2249951
F     0.4800686   -2.1979826    1.0306525
F     1.4498840   -0.4466933    1.8169091
C    -0.7583706   -0.4454200   -1.1683293
F    -1.9657060    0.0182422   -1.5031229
F    -0.7987444   -1.7809426   -1.3391010
F     0.1037229    0.0277087   -2.1023846

MP2 energy GEOOPT =  -1124.9141255699 H
SCF energy GEOOPT =  -1121.816961095 H
ZPE =   149.3 kJ/mol
FREEH energy =   178.49 kJ/mol
FREEH entropy =   0.42887 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                       -0.00         0.00000        -       -
     2                       -0.00         0.00000        -       -
     3                       -0.00         0.00000        -       -
     4                       -0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a             140.36         0.33315       YES     YES
     8        a             140.37         0.33319       YES     YES
     9        a             141.11         0.00248       YES     YES
    10        a             184.94         0.43422       YES     YES
    11        a             184.95         0.43447       YES     YES
    12        a             229.47         0.55404       YES     YES
    13        a             308.31         7.52124       YES     YES
    14        a             308.32         7.52072       YES     YES
    15        a             325.39         0.00148       YES     YES
    16        a             328.50         0.65728       YES     YES
    17        a             341.96         0.66508       YES     YES
    18        a             341.97         0.66471       YES     YES
    19        a             390.80         1.71910       YES     YES
    20        a             390.80         1.71928       YES     YES
    21        a             521.48         1.40828       YES     YES
    22        a             566.65         8.36304       YES     YES
    23        a             566.65         8.36297       YES     YES
    24        a             574.61         0.00082       YES     YES
    25        a             601.45         0.12796       YES     YES
    26        a             601.45         0.12795       YES     YES
```

27	a	688.15	4.27024	YES	YES
28	a	760.35	25.63395	YES	YES
29	a	760.35	25.63295	YES	YES
30	a	781.76	2.00593	YES	YES
31	a	1002.98	320.07956	YES	YES
32	a	1002.98	320.08878	YES	YES
33	a	1149.26	15.16220	YES	YES
34	a	1166.03	36.80136	YES	YES
35	a	1166.03	36.81213	YES	YES
36	a	1264.14	882.54816	YES	YES
37	a	1274.77	161.54658	YES	YES
38	a	1274.78	161.54567	YES	YES
39	a	1319.04	75.42294	YES	YES
40	a	1384.81	7.37551	YES	YES
41	a	1388.37	278.79492	YES	YES
42	a	1388.38	278.77368	YES	YES

$end

$NC_5F_4O^-$

Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:

N	-1.2737647	0.1715338	1.0281222
O	1.9496863	-0.2626068	-1.5736091
F	-0.0092145	1.5018204	2.3574285
F	2.1371699	1.2929876	0.7506625
C	0.9983057	0.6468157	0.4176572
C	0.9806114	-0.1320732	-0.7914972
F	-0.5115032	-1.5119557	-2.0628167
F	-2.5234073	-1.1607126	-0.3132640
C	-1.3341517	-0.5550792	-0.0737969
C	-0.1030962	0.7486519	1.2338702
C	-0.3106358	-0.7393819	-0.9727567

MP2 energy GEOOPT = -718.8939196011 H
SCF energy GEOOPT = -716.7170229081 H
ZPE = 133.9 kJ/mol
FREEH energy = 153.84 kJ/mol
FREEH entropy = 0.36465 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	170.38	0.00000	YES	YES
8	a	173.49	2.11520	YES	YES
9	a	284.18	2.95861	YES	YES
10	a	318.65	0.03911	YES	YES
11	a	331.66	0.00528	YES	YES
12	a	379.75	2.32010	YES	YES
13	a	380.48	0.01572	YES	YES
14	a	417.09	2.54509	YES	YES
15	a	478.15	0.00000	YES	YES
16	a	483.57	0.20923	YES	YES
17	a	497.67	5.30266	YES	YES
18	a	623.03	1.35344	YES	YES
19	a	740.13	1.36971	YES	YES
20	a	784.68	0.00000	YES	YES
21	a	796.64	3.67186	YES	YES
22	a	802.05	3.27753	YES	YES
23	a	865.55	26.22311	YES	YES

```
    24        a             991.52       286.60068       YES     YES
    25        a            1128.29         1.10819       YES     YES
    26        a            1174.92       307.98425       YES     YES
    27        a            1230.58       215.44092       YES     YES
    28        a            1347.75       106.96212       YES     YES
    29        a            1447.27        22.18996       YES     YES
    30        a            1557.45       476.36083       YES     YES
    31        a            1599.19       941.64248       YES     YES
    32        a            1658.81        30.26565       YES     YES
    33        a            1727.18       194.67814       YES     YES
$end
```

TeF_5O^-

```
Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
O     1.5192826   -0.1444628    1.1726129
Te    0.1161856   -0.0110479    0.0896752
F    -1.1852421    0.2412692    1.4229874
F    -0.3222870   -1.8389313    0.0486406
F    -1.3615583    0.1294661   -1.0508798
F     1.0482839   -0.2282460   -1.5286933
F     0.1853353    1.8519527   -0.1543430

MP2 energy GEOOPT =  -581.9360003394 H
SCF energy GEOOPT =  -580.2464190542 H
ZPE =   40.95 kJ/mol
FREEH energy =    59.90 kJ/mol
FREEH entropy =   0.35464 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000         -       -
     2                       0.00         0.00000         -       -
     3                       0.00         0.00000         -       -
     4                       0.00         0.00000         -       -
     5                       0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
     7        a            229.42         0.00006       YES     YES
     8        a            229.42         0.00006       YES     YES
     9        a            262.11         0.00000       YES     YES
    10        a            316.23         0.00000       YES     YES
    11        a            369.79        21.80070       YES     YES
    12        a            369.79        21.79908       YES     YES
    13        a            385.77        91.83148       YES     YES
    14        a            394.68        71.52915       YES     YES
    15        a            394.68        71.52775       YES     YES
    16        a            558.25         1.76347       YES     YES
    17        a            562.53         0.00000       YES     YES
    18        a            635.72       246.89322       YES     YES
    19        a            635.72       246.89324       YES     YES
    20        a            643.80        68.59725       YES     YES
    21        a            859.19        76.62610       YES     YES
$end
```

$C_{10}F_{15}O^-$

```
Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
C     0.2455033    0.4355422    1.7004865
C    -0.7990932    1.0741918    0.7632544
```

```
C     1.0526113   -0.6304164    0.9325286
F    -0.3628760   -0.1185933    2.7753887
F     1.0640824    1.3749925    2.2064531
C    -1.7544930   -0.0221843    0.2507688
C     0.0896293   -1.7198106    0.4193522
C    -0.9555978   -1.0900184   -0.5231559
F    -2.7109835    0.5110058   -0.5299127
F    -2.4185649   -0.5890776    1.2852965
F    -0.5231231   -2.3339553    1.4585692
F     0.7698487   -2.6933143   -0.2116939
C    -0.0800764    1.7330208   -0.4367145
F    -1.5252917    1.9888147    1.4763326
C     1.7685700    0.0312353   -0.2677175
F     1.9461869   -1.2068966    1.7936749
C    -0.2363158   -0.4276043   -1.7209936
F    -1.8187076   -2.0685462   -0.9353640
C     0.7814745    0.7193090   -1.3052172
F     0.7031641    2.7298438    0.0337294
F    -1.0111281    2.3374642   -1.2088732
F     2.5166896   -0.9100547   -0.8863700
F     2.6502764    0.9374132    0.2117326
F    -1.1756739    0.0617905   -2.5615514
F     0.4050363   -1.3933115   -2.4170602
O     1.3788523    1.2691597   -2.3029434

MP2 energy GEOOPT =  -1951.4329852417 H
SCF energy GEOOPT =  -1945.920756103 H
ZPE =   312.3 kJ/mol
FREEH energy =   360.57 kJ/mol
FREEH entropy =   0.54462 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a            167.20         0.56259       YES     YES
     8        a            167.20         0.56259       YES     YES
     9        a            171.32         0.00000       YES     YES
    10        a            229.01         0.02457       YES     YES
    11        a            229.01         0.02458       YES     YES
    12        a            235.22         0.41454       YES     YES
    13        a            242.30         0.11975       YES     YES
    14        a            242.30         0.11974       YES     YES
    15        a            276.21         0.00000       YES     YES
    16        a            285.12         0.04534       YES     YES
    17        a            285.12         0.04532       YES     YES
    18        a            289.69         0.00903       YES     YES
    19        a            289.69         0.00902       YES     YES
    20        a            290.24         0.00000       YES     YES
    21        a            297.28         3.29930       YES     YES
    22        a            304.54         3.15428       YES     YES
    23        a            304.55         3.15419       YES     YES
    24        a            316.62         0.00000       YES     YES
    25        a            323.18         1.54592       YES     YES
    26        a            324.80         2.72749       YES     YES
    27        a            324.80         2.72730       YES     YES
    28        a            335.72         2.59055       YES     YES
    29        a            335.72         2.59100       YES     YES
    30        a            348.42         0.54833       YES     YES
    31        a            348.42         0.54826       YES     YES
    32        a            388.56         0.00895       YES     YES
    33        a            413.52         0.00000       YES     YES
    34        a            416.40         0.04443       YES     YES
    35        a            416.40         0.04443       YES     YES
    36        a            430.66         0.94134       YES     YES
```

```
    37        a             430.66         0.94130       YES     YES
    38        a             451.42         0.33108       YES     YES
    39        a             478.10        14.15320       YES     YES
    40        a             478.10        14.15310       YES     YES
    41        a             481.73         9.32432       YES     YES
    42        a             600.91         1.63032       YES     YES
    43        a             644.77         0.22048       YES     YES
    44        a             644.77         0.22042       YES     YES
    45        a             686.17        14.01826       YES     YES
    46        a             686.17        14.01848       YES     YES
    47        a             686.82        11.11353       YES     YES
    48        a             730.89         0.40031       YES     YES
    49        a             920.44         2.39778       YES     YES
    50        a             920.44         2.39849       YES     YES
    51        a             926.76         0.00000       YES     YES
    52        a            1007.48       327.77874       YES     YES
    53        a            1007.48       327.88409       YES     YES
    54        a            1030.26       216.54834       YES     YES
    55        a            1030.26       216.53272       YES     YES
    56        a            1032.73       466.76682       YES     YES
    57        a            1086.63         2.51188       YES     YES
    58        a            1086.63         2.50995       YES     YES
    59        a            1151.75         0.00000       YES     YES
    60        a            1153.86         0.41669       YES     YES
    61        a            1153.87         0.41721       YES     YES
    62        a            1158.96         0.00001       YES     YES
    63        a            1235.51         3.31182       YES     YES
    64        a            1235.52         3.31161       YES     YES
    65        a            1291.15        33.79864       YES     YES
    66        a            1291.15        33.79683       YES     YES
    67        a            1304.02         0.00000       YES     YES
    68        a            1308.57        41.76534       YES     YES
    69        a            1337.09        63.42687       YES     YES
    70        a            1359.80       107.00121       YES     YES
    71        a            1359.80       107.01377       YES     YES
    72        a            1365.01       191.97933       YES     YES
    73        a            1388.44       133.70885       YES     YES
    74        a            1388.44       133.75349       YES     YES
    75        a            1402.73       214.99400       YES     YES
    76        a            1407.23       127.26323       YES     YES
    77        a            1422.66       116.92697       YES     YES
    78        a            1422.67       116.91296       YES     YES
$end
```

$C_2F_5^-$

```
Method: MP2/def-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
F    -0.1536352   -1.6283617    0.7969840
F     0.9644733    0.1481160    1.5356424
F    -0.6043318   -0.3259732   -1.5670656
F    -1.2917408    0.7382605    0.1797259
F     0.4850954    1.4049523   -0.8473055
C     0.7614346   -0.6230720    0.3458816
C    -0.1612956    0.2860781   -0.4438628

MP2 energy GEOOPT =  -574.7069228625 H
SCF energy GEOOPT =  -573.1473419820 H
ZPE =   62.52 kJ/mol
FREEH energy =    77.75 kJ/mol
FREEH entropy =   0.32416 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                       -0.00         0.00000        -       -
```

```
     2                      -0.00          0.00000        -       -
     3                      -0.00          0.00000        -       -
     4                       0.00          0.00000        -       -
     5                       0.00          0.00000        -       -
     6                       0.00          0.00000        -       -
     7         a           154.45          0.61366      YES     YES
     8         a           258.66          1.64662      YES     YES
     9         a           279.15          1.52414      YES     YES
    10         a           385.25          0.98867      YES     YES
    11         a           454.47          1.97560      YES     YES
    12         a           535.61          0.04213      YES     YES
    13         a           593.77          0.84635      YES     YES
    14         a           605.16          5.18321      YES     YES
    15         a           736.46         15.16004      YES     YES
    16         a           854.06        189.66751      YES     YES
    17         a           862.59         47.00953      YES     YES
    18         a           994.88        127.15419      YES     YES
    19         a          1148.03        372.09710      YES     YES
    20         a          1199.25        362.96534      YES     YES
    21         a          1391.04        176.72157      YES     YES
$end
```

PD (H^+ induced decomposition) and CuD (Cu^+ induced decomposition)

The intrinsic stability of a WCA towards attack of a hard or soft electrophile and to eliminate the contribution of the intrinsic stability of L^-, the isodesmic decomposition reactions were calculated, Scheme S- 3.

$$M(L)_n^- + H^+ \xrightarrow[BP86/SV(P)]{\Delta H = PD} M(L)_{n-1} + HL$$

$$M(L)_n^- + Cu^+ \xrightarrow[BP86/SV(P)]{\Delta H = CuD} M(L)_{n-1} + CuL$$

Scheme S- 3: Underlying reactions for calculating the PD and CuD.

The standard entropy in Table S- 9 of Cu^+ and H^+ were calculated with the Sackur-Tetrode equation.[32]

Table S- 9: Summary of thermodynamic data calculated at the BP86(D3BJ)/def-SV(P) level of theory (grid m3, 298.15 K) for the calculation of the H^+ induced decomposition (PD) and Cu^+ induced decomposition (CuD):

	E_{SCF} / H	E_{SCF} / kJ·mol^{-1}	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	$G°$ / kJ·mol^{-1}	$H°$ / kJ·mol^{-1}
Cu^+	-1640.22	-4306384.41	3.72	0.16064	-4306426.10	-4306378.21
H^+	0.00	0.00	3.72	0.10895	-26.29	6.20
$[Al(C_6F_5)_4]^-$	-3151.86	-8275217.15	613.86	1.05443	-8274915.19	-8274600.81
$[B(C_6F_5)_4]^-$	-2934.29	-7703974.93	624.23	0.97863	-7703640.00	-7703348.22
$[B(OCH(CF_3)_2)_4]^-$	-3179.83	-8348641.63	652.36	1.07771	-8348308.11	-8347986.79
$[Al(OC(CF_3)_3)_4]^-$	-4744.67	-12457137.25	721.13	1.33929	-12456812.95	-12456413.64
$[Al(OC_5F_4N)_4]^-$	-3120.30	-8192333.59	627.22	1.08267	-8192026.69	-8191703.90
$[B(OC_5F_4N)_4]^-$	-2902.67	-7620948.52	634.84	1.01136	-7620612.74	-7620311.20
$[Al(OTeF_5)_4]^-$	-2571.17	-6750602.73	265.95	1.07522	-6750654.88	-6750334.30
$[Ga(OTeF_5)_4]^-$	-4253.59	-11167790.50	263.06	1.06350	-11167842.04	-11167524.96

$[Al(OC_{10}F_{15})_4]^-$	-8053.02	-21143201.57	1389.24	1.84778	-21142360.77	-21141809.85
$[Ga(C_2F_5)_4]^-$	-4225.13	-11093074.62	344.32	0.84508	-11092979.78	-11092727.82
$Al(C_6F_5)_3$	-2424.39	-6365246.54	463.17	0.87140	-6365040.69	-6364780.89
$B(C_6F_5)_3$	-2206.83	-5794041.26	472.69	0.81730	-5793809.77	-5793566.09
$B(OCH(CF_3)_2)_3$	-2391.01	-6277606.11	497.71	0.88587	-6277370.04	-6277105.92
$Al(OC(CF_3)_3)_3$	-3619.01	-9501700.91	541.91	1.05638	-9501471.48	-9501156.52
$Al(OC_5F_4N)_3$	-2400.71	-6303057.10	470.46	0.81449	-6302827.00	-6302584.16
$B(OC_5F_4N)_3$	-2183.11	-5731765.27	482.91	0.84514	-5731531.86	-5731279.88
$Al(OTeF_5)_3$	-1988.88	-5221794.53	199.43	0.79318	-5221829.11	-5221592.62
$Ga(OTeF_5)_3$	-3671.29	-9638964.99	197.06	0.81575	-9639008.66	-9638765.45
$Al(OC_{10}F_{15})_3$	-6100.25	-16016196.81	1042.73	1.42939	-16015577.77	-16015151.60
$Ga(C_2F_5)_3$	-3649.97	-9582982.68	260.03	0.72732	-9582937.02	-9582720.17
CuC_6F_5	-2367.86	-6216810.18	153.09	0.43557	-6216784.48	-6216654.61
$CuOCH(CF_3)_2$	-2429.21	-6377902.72	158.63	0.44103	-6377873.10	-6377741.61
$CuOC(CF_3)_3$	-2766.02	-7262192.81	178.22	0.51191	-7262164.74	-7262012.11
$CuOC_5F_4N$	-2359.93	-6195992.13	154.71	0.43444	-6195964.47	-6195834.94
$CuOTeF_5$	-2222.66	-5835580.22	64.08	0.43246	-5835642.60	-5835513.66
$CuOC_{10}F_{15}$	-3593.11	-9433709.28	344.99	0.63684	-9433551.69	-9433361.81
CuC_2F_5	-2215.56	-5816940.59	86.34	0.37900	-5816964.77	-5816851.77
HC_6F_5	-727.91	-1911131.23	176.25	0.38843	-1911068.31	-1910952.50
$HOCH(CF_3)_2$	-789.26	-2072200.47	183.45	0.40282	-2072134.64	-2072014.54
$HOC(CF_3)_3$	-1126.06	-2956480.34	202.47	0.46753	-2956414.79	-2956275.40
HOC_5F_4N	-719.97	-1890273.73	178.93	0.38681	-1890207.65	-1890092.32
$HOTeF_5$	-582.67	-1529805.06	86.33	0.39010	-1529832.56	-1529716.25
$HOC_{10}F_{15}$	-1953.15	-5127982.70	369.11	0.59515	-5127788.55	-5127611.11
HC_2F_5	-575.62	-1511291.33	112.91	0.33605	-1511276.13	-1511175.94

Detailed results for the calculation of the PD and CuD

Note: The detailed results for the Lewis acids in Table S- 9 were already mentioned in a previous chapter (calculating the FIA pages 79-123) and therefore are not listed again. The detailed results for the anions in Table S- 9 were already mentioned in a previous chapter (calculating the LA pages 130-166) and therefore are not listed again.

CuC_6F_5

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: cs

Cartesian coordinates in Ångström:
C    -1.1475285   -0.8482463    0.0000000
C    -1.2540309    0.5528124    0.0000000
C    -0.1239196    1.3774963    0.0000000
```

```
C     1.1348797    0.7667983    0.0000000
C     1.2807841   -0.6308934    0.0000000
C     0.1290925   -1.4385344    0.0000000
F    -2.4944551    1.0869258    0.0000000
F    -2.2379476   -1.6272436    0.0000000
F     0.2479975   -2.7710368    0.0000000
F     2.4929245   -1.2040819    0.0000000
F     2.2586434    1.5150279    0.0000000
Cu   -0.2864399    3.2209757    0.0000000

SCF energy GEOOPT =  -2367.858071103 H
ZPE =   124.8 kJ/mol
FREEH energy =   153.09 kJ/mol
FREEH entropy =   0.43557 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                       -0.00         0.00000        -       -
     2                       -0.00         0.00000        -       -
     3                       -0.00         0.00000        -       -
     4                       -0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a"             77.60         3.99994       YES     YES
     8        a'             86.55         4.67603       YES     YES
     9        a"            121.96         0.00072       YES     YES
    10        a"            154.12         0.26605       YES     YES
    11        a"            201.73         0.00565       YES     YES
    12        a'            223.66         5.77513       YES     YES
    13        a'            261.33         0.04257       YES     YES
    14        a'            269.28         1.49350       YES     YES
    15        a'            299.85         0.17465       YES     YES
    16        a"            330.96         7.58799       YES     YES
    17        a'            344.53         0.39382       YES     YES
    18        a"            391.42         0.03711       YES     YES
    19        a'            430.17         0.08083       YES     YES
    20        a"            483.39         2.95195       YES     YES
    21        a'            485.25         0.27651       YES     YES
    22        a'            564.37         0.33007       YES     YES
    23        a"            570.39         3.59414       YES     YES
    24        a"            628.66         0.00521       YES     YES
    25        a'            725.13         0.23044       YES     YES
    26        a'            798.60        47.15831       YES     YES
    27        a'            966.32       159.61733       YES     YES
    28        a'           1079.19        96.29023       YES     YES
    29        a'           1141.88         2.45241       YES     YES
    30        a'           1275.12         0.22131       YES     YES
    31        a'           1359.59         0.05816       YES     YES
    32        a'           1377.06        26.05238       YES     YES
    33        a'           1477.80       481.36044       YES     YES
    34        a'           1506.67       230.73481       YES     YES
    35        a'           1615.48         6.08720       YES     YES
    36        a'           1617.59         0.71321       YES     YES
$end
```

$CuOCH(CF_3)_2$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
O    -0.5327216    1.4358973   -0.7109231
C     0.3213360    0.4908336   -0.2029086
C     0.2787347   -0.8322120   -1.0127641
F     1.1552082   -1.7541317   -0.5636404
F    -0.9646171   -1.4030874   -0.9703987
F     0.5578398   -0.5866740   -2.3060613
```

```
C     0.0932488    0.2554444    1.3131380
F    -1.1636137   -0.2288056    1.5572222
F     0.2062114    1.4187441    1.9800727
F     0.9683579   -0.6201288    1.8490332
H     1.3821216    0.8464393   -0.2854136
Cu   -2.3021060    0.9776807   -0.6473563

SCF energy GEOOPT =  -2429.214981847 H
ZPE =   130.8 kJ/mol
FREEH energy =   158.63 kJ/mol
FREEH entropy =   0.44103 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             36.90         0.10382       YES     YES
     8        a             65.71         8.10081       YES     YES
     9        a             71.66         2.60250       YES     YES
    10        a            104.52         8.04280       YES     YES
    11        a            163.33         0.10024       YES     YES
    12        a            236.99         1.03807       YES     YES
    13        a            251.32         6.44330       YES     YES
    14        a            291.81         0.25903       YES     YES
    15        a            315.94         0.26942       YES     YES
    16        a            340.37         3.53833       YES     YES
    17        a            457.19         0.66729       YES     YES
    18        a            499.93         1.79589       YES     YES
    19        a            512.94         2.65846       YES     YES
    20        a            531.52         0.63365       YES     YES
    21        a            534.92        17.77778       YES     YES
    22        a            602.49         2.85406       YES     YES
    23        a            667.66        44.81198       YES     YES
    24        a            726.17        10.38191       YES     YES
    25        a            826.47        43.20324       YES     YES
    26        a            854.50        20.42525       YES     YES
    27        a           1075.40       130.63676       YES     YES
    28        a           1154.01        99.87629       YES     YES
    29        a           1159.72        11.23721       YES     YES
    30        a           1178.28       548.69707       YES     YES
    31        a           1204.61       150.76404       YES     YES
    32        a           1226.97       351.84327       YES     YES
    33        a           1235.55        18.64328       YES     YES
    34        a           1323.10        11.13504       YES     YES
    35        a           1330.92       112.47551       YES     YES
    36        a           2888.42        38.85449       YES     YES
$end
```

$CuOC(CF_3)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
F     0.7344116    2.1853106   -1.0418365
F    -0.8488656    1.0902952   -2.0522089
F     1.1673017    0.2590183   -1.9683454
F     1.7592168   -1.3030212    0.2149588
F     2.1080469    0.7652033    0.8192726
F     0.9458487   -0.5583969    2.0944641
F    -2.2704949   -0.6199896   -0.5708090
F    -0.5453142   -1.8128530   -1.1653791
F    -1.1711895   -1.7471282    0.9289466
```

```
O    -0.7962717    1.1637188    0.8494295
C    -1.0363982   -1.0012234   -0.2127642
C     0.2432886    0.9602801   -1.2720870
C     1.2000168   -0.2246324    0.7916448
C    -0.1298180    0.2522759    0.0863965
Cu   -1.3597790    0.5911425    2.4983170

SCF energy GEOOPT =  -2766.023308616 H
ZPE =   140.7 kJ/mol
FREEH energy =   178.22 kJ/mol
FREEH entropy =   0.51191 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             44.97         0.24428       YES     YES
     8        a             50.31         4.47298       YES     YES
     9        a             67.48         3.11408       YES     YES
    10        a             76.81         2.12849       YES     YES
    11        a             90.12         5.36762       YES     YES
    12        a            148.90         4.34529       YES     YES
    13        a            156.31         0.04019       YES     YES
    14        a            180.22         0.47596       YES     YES
    15        a            222.30         3.47106       YES     YES
    16        a            262.81         5.16677       YES     YES
    17        a            285.25         0.07208       YES     YES
    18        a            293.01         1.36209       YES     YES
    19        a            310.69         0.61743       YES     YES
    20        a            316.04         0.31930       YES     YES
    21        a            327.26         0.24859       YES     YES
    22        a            345.30         3.01194       YES     YES
    23        a            465.61         2.78039       YES     YES
    24        a            513.60         4.43017       YES     YES
    25        a            518.77         3.43734       YES     YES
    26        a            522.26         1.45220       YES     YES
    27        a            536.24         2.23648       YES     YES
    28        a            551.40         0.64102       YES     YES
    29        a            564.07         2.75869       YES     YES
    30        a            677.82         0.95818       YES     YES
    31        a            702.90        39.03189       YES     YES
    32        a            713.52        33.68932       YES     YES
    33        a            748.09         4.14365       YES     YES
    34        a            947.99       127.06147       YES     YES
    35        a            958.92       150.44047       YES     YES
    36        a           1077.07         5.65133       YES     YES
    37        a           1131.00        14.37895       YES     YES
    38        a           1166.11        11.66509       YES     YES
    39        a           1174.24         3.91113       YES     YES
    40        a           1184.73       200.44419       YES     YES
    41        a           1201.92       212.81289       YES     YES
    42        a           1214.53       306.84607       YES     YES
    43        a           1250.18       505.36998       YES     YES
    44        a           1257.75       525.19217       YES     YES
    45        a           1266.18        92.48559       YES     YES
$end
```

$CuOC_5F_4N$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
```

```
O    -1.7031494   -0.0187659    1.4778850
C    -0.6816534   -0.0542134    0.6557151
C    -0.6030984    0.6796722   -0.5635816
C     0.5235643    0.5969746   -1.3816093
N     1.5684142   -0.1546977   -1.0876983
C     1.5360636   -0.8582215    0.0359068
C     0.4635370   -0.8598482    0.9345377
F     0.4910595   -1.5973869    2.0530082
F     2.6085576   -1.6113707    0.3165217
F     0.5612415    1.3070477   -2.5193585
F    -1.6677418    1.4792637   -0.9068916
Cu   -3.0967947    1.0915461    0.9855646

SCF energy GEOOPT =  -2359.928894258 H
ZPE =   127.1 kJ/mol
FREEH energy =   154.71 kJ/mol
FREEH entropy =   0.43444 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             47.59         4.67361       YES     YES
     8        a             98.29         9.44795       YES     YES
     9        a            115.41         0.03260       YES     YES
    10        a            136.18         3.04961       YES     YES
    11        a            197.24        10.25672       YES     YES
    12        a            206.41         2.94380       YES     YES
    13        a            281.09         0.07456       YES     YES
    14        a            302.97         1.16005       YES     YES
    15        a            328.55         1.19223       YES     YES
    16        a            351.92         0.07364       YES     YES
    17        a            411.51         0.29164       YES     YES
    18        a            433.86         0.81412       YES     YES
    19        a            456.62         1.21790       YES     YES
    20        a            528.98         3.63351       YES     YES
    21        a            587.07         2.86947       YES     YES
    22        a            616.94         1.26633       YES     YES
    23        a            625.73         3.37359       YES     YES
    24        a            627.86         3.50292       YES     YES
    25        a            672.65         2.88001       YES     YES
    26        a            737.01         0.92258       YES     YES
    27        a            960.19       173.59576       YES     YES
    28        a           1113.05       297.26288       YES     YES
    29        a           1132.47        32.91322       YES     YES
    30        a           1269.09         5.58961       YES     YES
    31        a           1369.65        71.53254       YES     YES
    32        a           1421.87        44.82667       YES     YES
    33        a           1486.58       474.40719       YES     YES
    34        a           1518.18       325.28355       YES     YES
    35        a           1592.75        27.90433       YES     YES
    36        a           1625.81       304.70798       YES     YES
$end
```

$CuOTeF_5$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Te   -0.3789695   -0.0316757   -0.0057672
O     0.9314476   -1.3498418    0.4931175
F     1.2319824    1.2078366   -0.3440483
```

```
F    -1.4935633    1.4440206   -0.5517312
F    -1.9378280   -1.1193460    0.2836628
F    -0.3563163   -0.5022256   -1.8913516
F    -0.5175426    0.7285515    1.7785812
Cu    2.5207897   -0.3773196    0.2375368

SCF energy GEOOPT =  -2222.655238726 H
ZPE =   36.63 kJ/mol
FREEH energy =    64.08 kJ/mol
FREEH entropy =   0.43246 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              44.28         2.62432       YES     YES
     8        a             109.52         0.02431       YES     YES
     9        a             145.35         8.12924       YES     YES
    10        a             153.51         0.10478       YES     YES
    11        a             192.05         5.09725       YES     YES
    12        a             200.72         8.96267       YES     YES
    13        a             228.29         0.09066       YES     YES
    14        a             257.75         4.75604       YES     YES
    15        a             267.32        20.55732       YES     YES
    16        a             272.03        20.37018       YES     YES
    17        a             273.62        23.36563       YES     YES
    18        a             462.04        49.32821       YES     YES
    19        a             512.17         5.69359       YES     YES
    20        a             555.64        12.12965       YES     YES
    21        a             575.14         3.84589       YES     YES
    22        a             621.40       116.01880       YES     YES
    23        a             622.06        85.83524       YES     YES
    24        a             631.82       103.25757       YES     YES
$end
```

$CuOC_{10}F_{15}$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C    -1.5369581   -0.0416794    0.4112724
C    -0.8870939   -1.4161305    0.7696268
C     0.5843211   -1.4585210    0.2492240
C     0.5914806   -1.2616950   -1.3020225
C    -0.0502189    0.1159572   -1.6628468
C    -1.5213845    0.1483945   -1.1405836
C     0.7715248    1.2690968   -0.9939099
C     1.3984533   -0.3065214    0.8984961
C    -0.7166473    1.1064574    1.0602160
C     0.7896268    1.1188634    0.5764444
F    -0.9136512   -1.6092431    2.1120387
F    -1.6034852   -2.4268003    0.2229120
F     1.1368883   -2.6715992    0.5539583
F    -0.0897807   -2.2684000   -1.9007568
F     1.8599828   -1.3259604   -1.7703956
F    -0.0518996    0.2693836   -3.0199325
F    -2.1113052    1.3223925   -1.4678985
F    -2.2504547   -0.8272067   -1.7348403
F    -2.8289737   -0.0228634    0.8570696
F     0.2335774    2.4624209   -1.3417724
F     2.0375136    1.2554498   -1.4750832
F     1.4242532   -0.4903580    2.2650977
```

```
F     2.6880024   -0.3620179    0.5022587
F    -1.2969710    2.2993619    0.8058628
F    -0.7527180    0.9640128    2.4313015
O     1.5032315    2.1240587    1.1270517
Cu    1.5926862    2.0331467    2.9672115

SCF energy GEOOPT =  -3593.110294566 H
ZPE =   285.5 kJ/mol
FREEH energy =   344.99 kJ/mol
FREEH entropy =   0.63684 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             43.91         5.97444       YES     YES
     8        a             71.65         6.27309       YES     YES
     9        a            128.68         3.21243       YES     YES
    10        a            129.76         0.59476       YES     YES
    11        a            132.60         0.05098       YES     YES
    12        a            169.75         4.09426       YES     YES
    13        a            190.06         0.00158       YES     YES
    14        a            195.20         0.43606       YES     YES
    15        a            201.02         0.00890       YES     YES
    16        a            203.80         0.36910       YES     YES
    17        a            209.71         1.56266       YES     YES
    18        a            225.75         0.04709       YES     YES
    19        a            240.80         0.01800       YES     YES
    20        a            243.44         0.33235       YES     YES
    21        a            243.90         0.08277       YES     YES
    22        a            246.66         0.19393       YES     YES
    23        a            249.24         2.24218       YES     YES
    24        a            250.39         0.85393       YES     YES
    25        a            253.83         1.57271       YES     YES
    26        a            257.63         0.66553       YES     YES
    27        a            261.13         0.08380       YES     YES
    28        a            282.05         4.42740       YES     YES
    29        a            295.32         1.20121       YES     YES
    30        a            295.74         3.16683       YES     YES
    31        a            299.06         4.15387       YES     YES
    32        a            302.16         0.63165       YES     YES
    33        a            305.67         3.68255       YES     YES
    34        a            360.18         0.25146       YES     YES
    35        a            373.77         0.01922       YES     YES
    36        a            375.68         0.35917       YES     YES
    37        a            376.05         0.40377       YES     YES
    38        a            379.78         3.01122       YES     YES
    39        a            384.06         4.48092       YES     YES
    40        a            400.73         0.68583       YES     YES
    41        a            426.68         5.40927       YES     YES
    42        a            429.17         9.36973       YES     YES
    43        a            434.03         6.64608       YES     YES
    44        a            528.77         5.87109       YES     YES
    45        a            585.60         0.07721       YES     YES
    46        a            587.87         0.54087       YES     YES
    47        a            593.60         6.62464       YES     YES
    48        a            630.13        14.03714       YES     YES
    49        a            634.19        12.88844       YES     YES
    50        a            635.69        13.94192       YES     YES
    51        a            684.97         0.60392       YES     YES
    52        a            831.99         0.01192       YES     YES
    53        a            833.84         0.09668       YES     YES
    54        a            838.80         0.35025       YES     YES
    55        a            947.90       256.22335       YES     YES
    56        a            952.20       204.15482       YES     YES
```

57	a	966.18	306.49433	YES	YES
58	a	972.65	70.01625	YES	YES
59	a	981.82	30.62845	YES	YES
60	a	1016.29	3.09024	YES	YES
61	a	1025.45	18.02162	YES	YES
62	a	1044.57	2.86588	YES	YES
63	a	1051.16	2.30256	YES	YES
64	a	1060.81	0.03489	YES	YES
65	a	1069.39	5.40634	YES	YES
66	a	1104.82	1.00787	YES	YES
67	a	1109.34	11.25554	YES	YES
68	a	1126.13	0.22651	YES	YES
69	a	1189.75	0.94495	YES	YES
70	a	1192.02	8.38528	YES	YES
71	a	1203.75	40.86220	YES	YES
72	a	1211.89	10.41589	YES	YES
73	a	1213.68	3.81381	YES	YES
74	a	1223.44	95.51508	YES	YES
75	a	1243.52	249.76765	YES	YES
76	a	1248.50	217.27471	YES	YES
77	a	1253.49	1.90905	YES	YES
78	a	1256.34	88.68598	YES	YES
79	a	1259.31	452.42995	YES	YES
80	a	1262.41	288.80940	YES	YES
81	a	1296.43	9.62821	YES	YES

$end

CuC_2F_5

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

Cu	-0.1235360	2.1657544	-0.6079739
F	1.4991501	0.4797384	0.8337903
F	-0.5722109	0.5727875	1.5874320
F	0.5704875	-0.7044222	-1.5012657
F	0.0713722	-1.7994435	0.3211460
F	-1.4698317	-0.6475343	-0.7126653
C	0.1884480	0.5987323	0.4474869
C	-0.1638792	-0.6656127	-0.3679503

SCF energy GEOOPT = -2215.555777101 H
ZPE = 65.64 kJ/mol
FREEH energy = 86.34 kJ/mol
FREEH entropy = 0.37900 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	53.20	0.93302	YES	YES
8	a	110.28	4.01901	YES	YES
9	a	184.11	1.91245	YES	YES
10	a	210.86	2.42292	YES	YES
11	a	262.84	7.34923	YES	YES
12	a	277.36	4.53420	YES	YES
13	a	354.75	0.29116	YES	YES
14	a	415.01	0.10097	YES	YES
15	a	523.00	1.42856	YES	YES
16	a	568.14	1.80208	YES	YES
17	a	590.55	6.07085	YES	YES
18	a	720.01	23.45990	YES	YES

```
    19        a             905.71       127.68160       YES     YES
    20        a            1072.91       100.17715       YES     YES
    21        a            1086.37       211.61782       YES     YES
    22        a            1182.61       163.27418       YES     YES
    23        a            1189.67       248.50680       YES     YES
    24        a            1267.00       313.48808       YES     YES
$end
```

HC_6F_5

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: cs

Cartesian coordinates in Ångström:
C    -1.1553278   -0.7881433    0.0000000
C    -1.2670774    0.6136175    0.0000000
C    -0.1281126    1.4271369    0.0000000
C     1.1372434    0.8287193    0.0000000
C     1.2779955   -0.5705845    0.0000000
C     0.1234744   -1.3744378    0.0000000
F    -2.4894035    1.1613918    0.0000000
F    -2.2437936   -1.5623305    0.0000000
F     0.2419937   -2.7039602    0.0000000
F     2.4875417   -1.1388746    0.0000000
F     2.2413503    1.5857839    0.0000000
H    -0.2258840    2.5216815    0.0000000

SCF energy GEOOPT =  -727.9114815409 H
ZPE =   152.7 kJ/mol
FREEH energy =   176.25 kJ/mol
FREEH entropy =   0.38843 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a"           127.47         0.00856       YES     YES
     8        a"           147.15         0.11738       YES     YES
     9        a"           201.87         1.44738       YES     YES
    10        a'           259.87         0.00998       YES     YES
    11        a'           261.68         0.02038       YES     YES
    12        a'           295.63         0.54075       YES     YES
    13        a"           313.88         0.00735       YES     YES
    14        a'           322.96         1.35787       YES     YES
    15        a"           390.51         0.00012       YES     YES
    16        a'           423.18         0.15299       YES     YES
    17        a'           460.21         0.41237       YES     YES
    18        a"           481.12         0.06433       YES     YES
    19        a"           547.32         2.18259       YES     YES
    20        a'           565.99         0.00637       YES     YES
    21        a"           631.18         0.00042       YES     YES
    22        a'           680.51         2.15669       YES     YES
    23        a'           704.01        17.71388       YES     YES
    24        a"           811.16        26.55101       YES     YES
    25        a'           951.93       138.57319       YES     YES
    26        a'          1080.99       150.88605       YES     YES
    27        a'          1146.69        52.25701       YES     YES
    28        a'          1178.69        25.47671       YES     YES
    29        a'          1287.37        10.01223       YES     YES
    30        a'          1357.88         5.46723       YES     YES
    31        a'          1419.75         6.86214       YES     YES
    32        a'          1517.01       170.88063       YES     YES
    33        a'          1536.99       420.21968       YES     YES
```

```
    34        a'          1633.21        36.94241       YES     YES
    35        a'          1644.50         8.04327       YES     YES
    36        a'          3153.60         4.11562       YES     YES
$end
```

$HOCH(CF_3)_2$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
O    -0.8297394    1.2838989   -0.7231533
C     0.2014767    0.4766251   -0.2227347
C     0.2859576   -0.8552339   -1.0032917
F     1.3365499   -1.6057178   -0.6199595
F    -0.8454943   -1.5832838   -0.8264192
F     0.4105273   -0.6024187   -2.3192494
C     0.0412538    0.2942257    1.3035667
F    -1.2053407   -0.1611726    1.5905475
F     0.1960971    1.4796044    1.9225090
F     0.9336916   -0.5706817    1.8203350
H     1.1571158    1.0143323   -0.3923175
H    -1.6820954    0.8298220   -0.5298328

SCF energy GEOOPT =  -789.2595189769 H
ZPE =   159.2 kJ/mol
FREEH energy =   183.45 kJ/mol
FREEH entropy =   0.40282 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              29.28         0.12394       YES     YES
     8        a              84.10         0.29758       YES     YES
     9        a             161.26         0.82764       YES     YES
    10        a             217.74         7.53387       YES     YES
    11        a             238.85         2.42093       YES     YES
    12        a             281.54         8.72180       YES     YES
    13        a             316.80         0.30867       YES     YES
    14        a             331.89         7.46625       YES     YES
    15        a             418.05       104.97693       YES     YES
    16        a             446.88         8.86036       YES     YES
    17        a             501.02         5.87921       YES     YES
    18        a             517.43         3.29667       YES     YES
    19        a             536.79         4.95056       YES     YES
    20        a             593.63         2.23569       YES     YES
    21        a             672.29        58.66034       YES     YES
    22        a             720.31        11.81377       YES     YES
    23        a             815.21        37.14656       YES     YES
    24        a             881.70        43.88981       YES     YES
    25        a            1094.44       140.10728       YES     YES
    26        a            1101.22       111.01454       YES     YES
    27        a            1169.96        17.50219       YES     YES
    28        a            1192.29       336.59186       YES     YES
    29        a            1226.42       143.85669       YES     YES
    30        a            1233.04       264.49465       YES     YES
    31        a            1250.06       173.58859       YES     YES
    32        a            1285.73       172.44082       YES     YES
    33        a            1349.34       117.76088       YES     YES
    34        a            1394.29         8.73188       YES     YES
    35        a            3035.74         3.54097       YES     YES
    36        a            3518.94        41.30487       YES     YES
```

```
$end
```

$HOC(CF_3)_3$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
F     0.6237602    2.2168136   -0.9264664
F    -0.9254477    1.1006536   -1.9652876
F     1.1156609    0.3306247   -1.9118501
F     1.7028080   -1.3573141    0.2956148
F     2.1155851    0.7296657    0.7716000
F     0.9180808   -0.4728450    2.1345560
F    -2.2914438   -0.6548604   -0.4851148
F    -0.5677586   -1.7947236   -1.1839343
F    -1.1196349   -1.8098510    0.9346187
O    -0.8298762    1.1040310    0.9426645
C    -1.0458597   -1.0404071   -0.1802243
C     0.1757889    0.9862394   -1.2008855
C     1.1870050   -0.2384489    0.8240454
C    -0.1422542    0.2088229    0.1181993
H    -0.9164139    0.6915991    1.8324643

SCF energy GEOOPT =  -1126.063952777 H
ZPE =   169.1 kJ/mol
FREEH energy =   202.47 kJ/mol
FREEH entropy =   0.46753 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)      km/mol          IR     RAMAN
     1                      -0.00        0.00000        -       -
     2                      -0.00        0.00000        -       -
     3                      -0.00        0.00000        -       -
     4                       0.00        0.00000        -       -
     5                       0.00        0.00000        -       -
     6                       0.00        0.00000        -       -
     7        a             56.73        0.05830       YES     YES
     8        a             64.86        0.18839       YES     YES
     9        a             71.31        0.07894       YES     YES
    10        a            156.44        0.20607       YES     YES
    11        a            159.20        0.64264       YES     YES
    12        a            182.05        1.93391       YES     YES
    13        a            258.87        1.43944       YES     YES
    14        a            269.86        4.68051       YES     YES
    15        a            283.28        8.75215       YES     YES
    16        a            302.95       32.47511       YES     YES
    17        a            313.56        6.98773       YES     YES
    18        a            321.09        0.17026       YES     YES
    19        a            332.02       20.67343       YES     YES
    20        a            348.30        2.25727       YES     YES
    21        a            376.91       62.67011       YES     YES
    22        a            472.66        6.40590       YES     YES
    23        a            518.98        7.59035       YES     YES
    24        a            521.09        5.19075       YES     YES
    25        a            526.32        2.37320       YES     YES
    26        a            554.24        0.68848       YES     YES
    27        a            556.47        0.25086       YES     YES
    28        a            634.97        2.32085       YES     YES
    29        a            707.97       44.28426       YES     YES
    30        a            709.53       39.52625       YES     YES
    31        a            751.29        1.17821       YES     YES
    32        a            933.69      128.26132       YES     YES
    33        a            968.31      143.76361       YES     YES
    34        a           1112.56        1.93825       YES     YES
    35        a           1145.99      253.02271       YES     YES
    36        a           1160.88       19.22749       YES     YES
```

37	a	1178.79	6.15630	YES	YES
38	a	1190.16	76.04753	YES	YES
39	a	1193.45	65.87283	YES	YES
40	a	1232.41	341.05035	YES	YES
41	a	1255.54	372.57459	YES	YES
42	a	1267.56	545.55720	YES	YES
43	a	1282.62	185.32031	YES	YES
44	a	1362.09	85.66703	YES	YES
45	a	3528.37	66.02875	YES	YES

$end

HOC_5F_4N

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

O	-1.8554550	0.0515483	1.3449300
C	-0.7491207	-0.0046753	0.5782169
C	-0.6171236	0.7506526	-0.6069948
C	0.5607859	0.6456567	-1.3556139
N	1.5634116	-0.1362369	-0.9981643
C	1.4579392	-0.8519426	0.1084514
C	0.3299157	-0.8377432	0.9450980
F	0.2653529	-1.5794595	2.0545200
F	2.4896413	-1.6310981	0.4430346
F	0.6879207	1.3586989	-2.4782000
F	-1.6492621	1.5476687	-0.9630622
H	-2.4840058	0.6869306	0.9277841

SCF energy GEOOPT = -719.9672773510 H
ZPE = 155.6 kJ/mol
FREEH energy = 178.93 kJ/mol
FREEH entropy = 0.38681 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	114.24	0.06276	YES	YES
8	a	148.85	0.15051	YES	YES
9	a	205.68	0.30221	YES	YES
10	a	260.31	6.24955	YES	YES
11	a	263.38	0.61574	YES	YES
12	a	308.60	3.14901	YES	YES
13	a	333.97	0.00399	YES	YES
14	a	340.16	1.11783	YES	YES
15	a	422.79	7.97824	YES	YES
16	a	446.95	0.15761	YES	YES
17	a	466.81	0.98543	YES	YES
18	a	474.98	107.63062	YES	YES
19	a	587.58	0.47555	YES	YES
20	a	591.39	0.60509	YES	YES
21	a	628.16	1.39165	YES	YES
22	a	639.95	3.11847	YES	YES
23	a	676.54	1.62203	YES	YES
24	a	721.92	6.07179	YES	YES
25	a	946.23	172.58632	YES	YES
26	a	1095.29	240.17521	YES	YES
27	a	1151.54	29.12051	YES	YES
28	a	1266.78	100.68208	YES	YES
29	a	1287.58	57.17439	YES	YES
30	a	1406.63	16.61500	YES	YES

```
    31        a            1433.56        35.21504       YES     YES
    32        a            1495.70       567.14983       YES     YES
    33        a            1528.85       141.05594       YES     YES
    34        a            1632.21       160.27278       YES     YES
    35        a            1644.61         6.83234       YES     YES
    36        a            3499.51       105.58947       YES     YES
$end
```

$HOTeF_5$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
Te   -0.2684007    0.1164629   -0.0446999
O     1.0006243   -1.2916459    0.4592194
F     1.2045389    1.3124738   -0.4170099
F    -1.5213801    1.4783748   -0.5346757
F    -1.6944560   -1.0980300    0.3366468
F    -0.2744513   -0.4252279   -1.8886729
F    -0.3520368    0.8094509    1.7466266
H     1.9055618   -0.9018587    0.3425656

SCF energy GEOOPT =  -582.6720067689 H
ZPE =   62.58 kJ/mol
FREEH energy =    86.33 kJ/mol
FREEH entropy =   0.39010 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a            146.90         1.05801       YES     YES
     8        a            155.71         1.05444       YES     YES
     9        a            165.03         9.14939       YES     YES
    10        a            187.21        42.48295       YES     YES
    11        a            241.39         7.79574       YES     YES
    12        a            255.11         3.55837       YES     YES
    13        a            262.69        31.92170       YES     YES
    14        a            271.37        24.00978       YES     YES
    15        a            273.94        35.86116       YES     YES
    16        a            283.88        84.81697       YES     YES
    17        a            576.89         1.44012       YES     YES
    18        a            592.00         4.59836       YES     YES
    19        a            593.81         2.95877       YES     YES
    20        a            645.67        82.28255       YES     YES
    21        a            652.53       113.02082       YES     YES
    22        a            656.38        93.62171       YES     YES
    23        a           1030.86       104.30224       YES     YES
    24        a           3471.45       122.15399       YES     YES
$end
```

$HOC_{10}F_{15}$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C    -1.5415410   -0.0494320    0.4309783
C    -0.8949586   -1.4303692    0.7757056
C     0.5811909   -1.4675198    0.2645933
```

```
C     0.6020912   -1.2465035   -1.2837976
C    -0.0352694    0.1399298   -1.6267703
C    -1.5132016    0.1649249   -1.1181077
C     0.7839226    1.2841379   -0.9330656
C     1.3936445   -0.3229710    0.9394290
C    -0.7220838    1.0909674    1.1054358
C     0.7686949    1.0801466    0.6152732
F    -0.9276512   -1.6361004    2.1141105
F    -1.6074865   -2.4317366    0.2100307
F     1.1359168   -2.6777245    0.5607153
F    -0.0771731   -2.2397643   -1.9031742
F     1.8730651   -1.3017495   -1.7444647
F    -0.0180557    0.3250271   -2.9768587
F    -2.0966819    1.3443518   -1.4343759
F    -2.2333920   -0.8015956   -1.7339111
F    -2.8312105   -0.0271148    0.8725213
F     0.2513995    2.4843411   -1.2586174
F     2.0541436    1.2792253   -1.3976507
F     1.4155422   -0.4902922    2.2935601
F     2.6819670   -0.3667831    0.5354731
F    -1.2922898    2.2886140    0.8469214
F    -0.7389693    0.9488392    2.4624241
O     1.4998207    2.1032657    1.2047520
H     1.4885653    1.9558857    2.1788704

SCF energy GEOOPT =  -1953.145563067 H
ZPE =   313.6 kJ/mol
FREEH energy =   369.11 kJ/mol
FREEH entropy =   0.59515 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a            131.12         0.05176       YES     YES
     8        a            131.77         0.08425       YES     YES
     9        a            132.96         0.18632       YES     YES
    10        a            193.21         0.08561       YES     YES
    11        a            193.56         0.34546       YES     YES
    12        a            196.95         1.87215       YES     YES
    13        a            197.61         0.70594       YES     YES
    14        a            202.93         0.08124       YES     YES
    15        a            218.97         8.13872       YES     YES
    16        a            230.20        12.08216       YES     YES
    17        a            240.35         0.41902       YES     YES
    18        a            241.38         0.71834       YES     YES
    19        a            242.62         0.08891       YES     YES
    20        a            243.52         0.07746       YES     YES
    21        a            248.51         2.01854       YES     YES
    22        a            249.27         0.91975       YES     YES
    23        a            252.08         0.84044       YES     YES
    24        a            258.33         3.16833       YES     YES
    25        a            261.07         3.67410       YES     YES
    26        a            265.43         3.98825       YES     YES
    27        a            294.22         4.87740       YES     YES
    28        a            295.38         8.50667       YES     YES
    29        a            296.71         5.79849       YES     YES
    30        a            298.30         4.46896       YES     YES
    31        a            299.75         2.32306       YES     YES
    32        a            328.00        53.34753       YES     YES
    33        a            362.56         0.00607       YES     YES
    34        a            377.18         0.13408       YES     YES
    35        a            378.06         0.35432       YES     YES
    36        a            378.46         0.02411       YES     YES
    37        a            389.75         6.05356       YES     YES
```

```
    38        a             393.46        20.19706       YES     YES
    39        a             395.89         8.11800       YES     YES
    40        a             431.01         6.59713       YES     YES
    41        a             432.15        11.58289       YES     YES
    42        a             432.80        16.42289       YES     YES
    43        a             555.78         0.90161       YES     YES
    44        a             589.19         0.34320       YES     YES
    45        a             589.61         0.14262       YES     YES
    46        a             634.82        16.45322       YES     YES
    47        a             635.68        12.93569       YES     YES
    48        a             636.55        12.49655       YES     YES
    49        a             684.04         0.63434       YES     YES
    50        a             821.95        17.61903       YES     YES
    51        a             833.79         0.01560       YES     YES
    52        a             834.66         0.00568       YES     YES
    53        a             935.05       221.20185       YES     YES
    54        a             959.95       282.17274       YES     YES
    55        a             964.93       258.35610       YES     YES
    56        a             983.24        55.36513       YES     YES
    57        a             984.58         5.79269       YES     YES
    58        a            1042.71        17.52682       YES     YES
    59        a            1044.12         6.53834       YES     YES
    60        a            1051.94         0.06966       YES     YES
    61        a            1054.82         2.93235       YES     YES
    62        a            1056.14         8.66503       YES     YES
    63        a            1060.83         0.05134       YES     YES
    64        a            1123.57         0.32835       YES     YES
    65        a            1126.01         7.12005       YES     YES
    66        a            1133.47         0.52535       YES     YES
    67        a            1184.43       113.81252       YES     YES
    68        a            1201.22         3.74311       YES     YES
    69        a            1207.37         3.39163       YES     YES
    70        a            1211.06         2.73688       YES     YES
    71        a            1213.53         1.56144       YES     YES
    72        a            1236.61        88.78908       YES     YES
    73        a            1242.92       179.88031       YES     YES
    74        a            1250.57       307.35572       YES     YES
    75        a            1261.37       436.32422       YES     YES
    76        a            1263.99       143.04858       YES     YES
    77        a            1264.52        38.75120       YES     YES
    78        a            1266.25       164.67529       YES     YES
    79        a            1295.97         2.08597       YES     YES
    80        a            1351.18        51.54047       YES     YES
    81        a            3519.26        70.53879       YES     YES
$end
```

HC_2F_5

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
H    -0.0261720    1.5698871   -0.2553170
F     1.4752594    0.6410426    0.7291098
F    -0.6004769    0.7288945    1.4921335
F     0.5683226   -0.6759838   -1.5249044
F     0.0672356   -1.7129834    0.3351971
F    -1.4763644   -0.6052271   -0.7500817
C     0.1664996    0.6725069    0.3756349
C    -0.1743039   -0.6181368   -0.4017723

SCF energy GEOOPT =  -575.6204965163 H
ZPE =   96.58 kJ/mol
FREEH energy =   112.91 kJ/mol
FREEH entropy =   0.33605 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
```

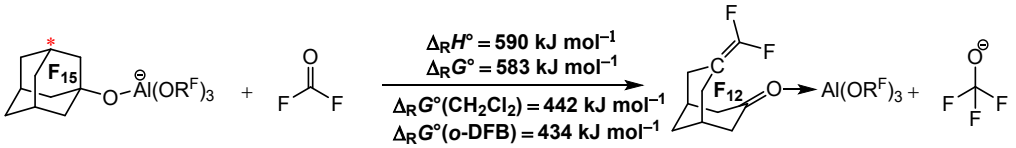
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	68.61	0.63867	YES	YES
8	a	203.44	2.46081	YES	YES
9	a	235.41	3.38180	YES	YES
10	a	351.64	0.02077	YES	YES
11	a	401.74	0.83717	YES	YES
12	a	507.71	6.31236	YES	YES
13	a	565.13	13.27041	YES	YES
14	a	566.58	0.52532	YES	YES
15	a	707.10	30.24840	YES	YES
16	a	850.23	43.31795	YES	YES
17	a	1128.28	112.77522	YES	YES
18	a	1132.78	88.35604	YES	YES
19	a	1178.28	211.28060	YES	YES
20	a	1203.88	380.69833	YES	YES
21	a	1284.25	169.76517	YES	YES
22	a	1356.25	17.99930	YES	YES
23	a	1406.39	0.40632	YES	YES
24	a	2999.20	32.29332	YES	YES

$end

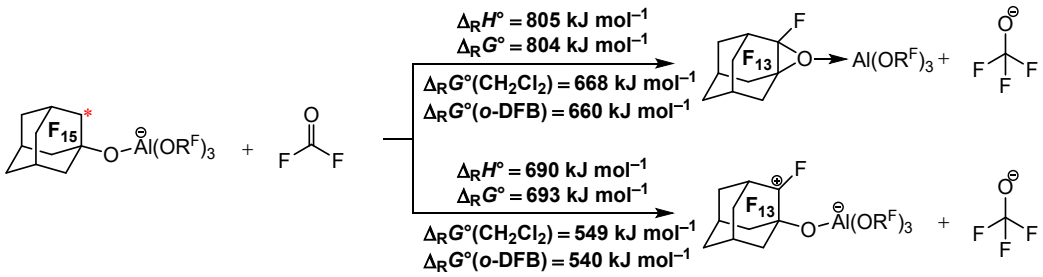
Fluoride Ion Abstraction from [*pfAd*]$^-$ vs. [Al(OR^F)$_4$]$^-$

While the FIA and LA allow a statement regarding the thermodynamic stability towards removal of a univalent ligand, the susceptibility of the fluorinated ligands in the [*pf*]$^-$ and the novel [*pfAd*]$^-$ anion themselves towards fluoride abstraction were calculated additionally (BP86/D3(BJ)/def-SV(P) level).

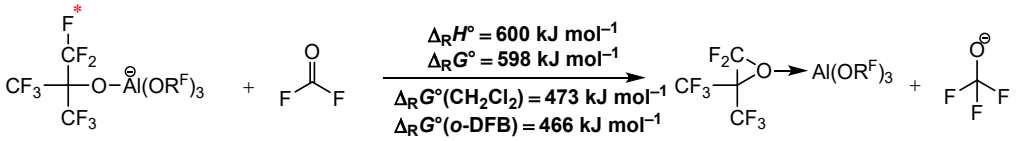
(1) Fluoride abstraction from a CF group of the [*pfAd*]$^-$ anion



(2) Fluoride abstraction from a CF$_2$ group of the [*pfAd*]$^-$ anion



(3) Fluoride abstraction from a CF$_3$ group of the [*pf*]$^-$ anion



Scheme S- 4: : Calculated reaction enthalpy $\Delta_R H°$ and Gibbs free energy $\Delta_R G°$ for the decomposition of the [Al(OR^F)$_4$]$^-$ WCAs ((1) and (2) R^F = C$_{10}$F$_{15}$), (3) R^F = C(CF$_3$)$_3$) under fluoride abstraction (BP86/def-SV(P) level with D3(BJ) dispersion). Solvation effects on the Gibbs free energy $\Delta_R G°$ were calculated by use of the COSMO solvation model for CH$_2$Cl$_2$ (ε = 8.93[33]) and *o*-DFB (ε =13.38[33]). The red star marks the abstracted fluoride ion. The experimental FIA of COF$_2$ of 209 kJ mol^{-1} was used as an anchor point for comparison.

Table S- 10: Summary of thermodynamic data calculated at the BP86(D3BJ)/def-SV(P) level of theory (grid m3, 298.15 K) for the calculation of possible fluoride abstraction which could lead to decomposition of the anion.

	E_{SCF} / H	E_{SCF} / kJ·mol^{-1}	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	$G°$ / kJ·mol^{-1}	$H°$ / kJ·mol^{-1}
COF_2	-312.80	-821269.30	44.88	0.26559	-821301.12	-821221.94
COF_3^-	-412.64	-1083386.45	51.61	0.28667	-1083417.83	-1083332.36
$[Al(OC_{10}F_{15})_4]^-$	-8053.02	-21143201.57	1389.24	1.84778	-21142360.77	-21141809.85
$Al(OC_{10}F_{15})_3{\cdot}OC_{10}F_{14}$ (1)	-7953.04	-20880701.57	1380.79	1.85096	-20879870.17	-20879318.30
$Al(OC_{10}F_{15})_3{\cdot}OC_{10}F_{14}$ (2, epoxid)	-7952.96	-20880483.74	1377.70	1.82934	-20879648.98	-20879103.57
$Al(OC_{10}F_{15})_3{\cdot}OC_{10}F_{14}$ (2, zwitterionic)	-7953.00	-20880597.43	1376.82	1.81847	-20879760.30	-20879218.13
$[Al(OC(CF_3)_3)_4]^-$	-4744.67	-12457137.25	721.13	1.33929	-12456812.95	-12456413.64
$[Al(OC(CF_3)_3)_3{\cdot}OCF_2C(CF_3)_2$	-4644.69	-12194626.23	711.58	1.32480	-12194307.16	-12193912.18

Table S- 11: Summary of thermodynamic data calculated at the BP86(D3BJ)/def-SV(P) level of theory (grid m3, 298.15 K) with additional single point COSMO model in CH_2Cl_2 (8.93[33]) for the calculation of possible fluoride abstraction which could lead to decomposition of the anion.

	E_{SCF} / H	E_{SCF} / kJ·mol^{-1}	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	$G°$ / kJ·mol^{-1}	$H°$ / kJ·mol^{-1}
COF_2	-312.81	-821277.29	44.88	0.26559	-821309.12	-821229.93
COF_3^-	-412.73	-1083615.33	51.61	0.28667	-1083646.71	-1083561.24
$[Al(OC_{10}F_{15})_4]^-$	-8053.06	-21143293.17	1389.24	1.84778	-21142452.36	-21141901.45
$Al(OC_{10}F_{15})_3{\cdot}OC_{10}F_{14}$ (1)	-7953.04	-20880712.99	1380.79	1.85096	-20879881.58	-20879329.72
$Al(OC_{10}F_{15})_3{\cdot}OC_{10}F_{14}$ (2, epoxid)	-7952.96	-20880490.10	1377.70	1.82934	-20879655.33	-20879109.92
$Al(OC_{10}F_{15})_3{\cdot}OC_{10}F_{14}$ (2, zwitterionic)	-7953.01	-20880612.36	1376.82	1.81847	-20879775.24	-20879233.06
$[Al(OC(CF_3)_3)_4]^-$	-4744.71	-12457244.26	721.13	1.33929	-12456919.96	-12456520.65
$[Al(OC(CF_3)_3)_3{\cdot}OCF_2C(CF_3)_2$	-4644.69	-12194637.18	711.58	1.32480	-12194318.11	-12193923.12

Table S- 12: Summary of thermodynamic data calculated at the BP86(D3BJ)/def-SV(P) level of theory (grid m3, 298.15 K) with additional single point COSMO model in *o*-DFB (13.38[33]) for the calculation of possible fluoride abstraction which could lead to decomposition of the anion.

	E_{SCF} / H	E_{SCF} / kJ·mol^{-1}	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	$G°$ / kJ·mol^{-1}	$H°$ / kJ·mol^{-1}
COF_2	-312.81	-821277.82	44.88	0.26559	-821309.65	-821230.46
COF_3^-	-412.73	-1083629.25	51.61	0.28667	-1083660.63	-1083575.16
$[Al(OC_{10}F_{15})_4]^-$	-8053.06	-21143298.81	1389.24	1.84778	-21142458.01	-21141907.09
$Al(OC_{10}F_{15})_3{\cdot}OC_{10}F_{14}$ (1)	-7952.96	-20880490.50	1377.70	1.82934	-20879655.74	-20879110.33
$Al(OC_{10}F_{15})_3{\cdot}OC_{10}F_{14}$ (2, epoxid)	-7953.01	-20880613.40	1376.82	1.81847	-20879776.28	-20879234.10
$Al(OC_{10}F_{15})_3{\cdot}OC_{10}F_{14}$ (2, zwitterionic)	-7953.04	-20880713.76	1380.79	1.85096	-20879882.36	-20879330.49
$[Al(OC(CF_3)_3)_4]^-$	-4744.72	-12457250.77	721.13	1.33929	-12456926.47	-12456527.16
$[Al(OC(CF_3)_3)_3{\cdot}OCF_2C(CF_3)_2$	-4644.69	-12194637.90	711.58	1.32480	-12194318.83	-12193923.84

Detailed results for the calculation of the Fluoride Ion Abstraction from [*pfAd*]$^-$ vs. [Al(OR^F)$_4$]$^-$ without COSMO model

COF_2

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: cs

Cartesian coordinates in Ångström:
C         -0.06981        0.06516        0.00000
O         -0.93579        0.87381        0.00000
F         -0.22929       -1.25369        0.00000
F          1.23490        0.31472        0.00000

SCF energy GEOOPT =  -312.8049721102 H
ZPE =   36.15 kJ/mol
FREEH energy =    44.88 kJ/mol
FREEH entropy =   0.26559 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a'            566.13         4.83594       YES     YES
     8        a'            600.85         4.97275       YES     YES
     9        a"            746.20        28.32177       YES     YES
    10        a'            947.55        49.98302       YES     YES
    11        a'           1226.96       404.95850       YES     YES
    12        a'           1955.42       411.54023       YES     YES
$end
```

COF_3^-

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C         -0.09521        0.09170       -0.07555
O         -0.86080        0.82884       -0.68195
F         -0.68327       -0.96485        0.71655
F          0.77957        0.70350        0.89931
F          0.85972       -0.65918       -0.85836

SCF energy GEOOPT =  -412.6401278204 H
ZPE =   40.51 kJ/mol
FREEH energy =    51.61 kJ/mol
FREEH entropy =   0.28667 kJ/mol/K

$vibrational spectrum
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#                         cm**(-1)        km/mol          IR     RAMAN
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     2                      -0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a            394.79         0.07382       YES     YES
     8        a            395.40         0.06561       YES     YES
     9        a            534.58        19.71310       YES     YES
    10        a            535.20        19.85267       YES     YES
    11        a            561.77         0.08048       YES     YES
    12        a            783.90        70.16911       YES     YES
    13        a            924.53       383.54574       YES     YES
    14        a            928.21       383.57078       YES     YES
    15        a           1714.87       610.18473       YES     YES
$end
```

$[Al(OC_{10}F_{15})_4]^-$

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C         -1.04186       -1.44280        5.61856
C         -2.10287       -0.79837        4.67378
C         -0.22935       -2.52018        4.83753
F         -1.65123       -2.00567        6.69589
F         -0.21055       -0.49363        6.11077
C         -3.07176       -1.90428        4.15315
C         -1.20254       -3.62426        4.32201
C         -2.26330       -2.98441        3.37207
F         -4.02046       -1.36236        3.35412
F         -3.73242       -2.47702        5.19399
F         -1.81952       -4.23409        5.36853
F         -0.51445       -4.59453        3.67619
C         -1.37998       -0.13297        3.46005
F         -2.81619        0.13849        5.37062
C          0.49303       -1.85012        3.62334
F          0.69092       -3.08453        5.67939
C         -1.53217       -2.31948        2.16450
F         -3.11845       -3.95636        2.93028
C         -0.54062       -1.18558        2.63262
F         -0.57089        0.85571        3.91298
F         -2.30274        0.45859        2.66446
F          1.22994       -2.78286        2.97394
F          1.36546       -0.92288        4.08714
F         -2.44949       -1.80369        1.30772
```

F	-0.86083	-3.27390	1.47863
O	0.11564	-0.61464	1.61226
F	3.91310	1.10585	-0.98726
F	5.55864	1.61672	0.95071
F	3.30027	0.40090	1.48063
F	5.35596	3.47306	-1.12114
C	3.29372	2.28879	-0.75853
F	2.82586	2.72108	-1.95368
O	1.21624	1.22425	-0.26618
C	4.92249	2.79846	1.13276
C	4.34042	3.31611	-0.21724
C	2.71659	1.61440	1.62546
C	2.09870	2.08814	0.25240
F	5.85952	3.66387	1.60379
F	4.28614	2.18572	3.35234
C	3.76996	2.63423	2.16827
F	1.74432	1.47474	2.55542
C	3.64677	4.69281	0.01622
F	3.17091	5.18184	-1.15259
C	1.44822	3.50481	0.50037
F	0.92973	3.98669	-0.65393
F	4.55035	5.60418	0.46589
C	3.07617	4.01247	2.39832
C	2.48972	4.53137	1.05097
F	0.41692	3.39237	1.37529
F	3.96848	4.90815	2.89875
F	2.09668	3.90049	3.32522
F	1.89550	5.74743	1.25268
F	-1.75509	0.00507	-2.93076
F	-2.30900	1.95175	-4.51618
F	-0.93185	2.42591	-2.34402
F	-4.20066	-0.06860	-4.19916
C	-2.87875	0.25031	-2.21793
F	-3.30093	-0.93829	-1.72528
O	-1.66467	0.77211	-0.16564
C	-3.43840	2.16270	-3.80125
C	-3.95813	0.82319	-3.19092
C	-2.09995	2.61028	-1.67831
C	-2.56776	1.24896	-1.03527
F	-4.35119	2.66259	-4.67626
F	-2.72953	4.36599	-3.19604
C	-3.16972	3.18821	-2.65718
F	-1.85628	3.52106	-0.70586
C	-5.27843	1.08538	-2.40740
F	-5.76201	-0.07428	-1.90311
C	-3.92942	1.52625	-0.28735
F	-4.39941	0.38269	0.26603
F	-6.23769	1.56120	-3.24593
C	-4.49522	3.44431	-1.87505
C	-5.00959	2.10638	-1.26002
F	-3.73647	2.40068	0.72956
F	-5.43363	3.97008	-2.70742
F	-4.30052	4.36475	-0.90205
F	-6.17530	2.34222	-0.58196
F	0.47578	-1.00158	-3.98584
F	0.50895	-3.30520	-5.17798
F	-0.99934	-2.98701	-3.08646
F	2.87580	-1.84413	-5.06876
C	1.46573	-1.42507	-3.16317
F	2.19131	-0.32860	-2.83793
O	0.04977	-1.23160	-1.20619
C	1.51748	-3.67507	-4.35317
C	2.36847	-2.43317	-3.94260
C	0.04297	-3.35140	-2.30046
C	0.85874	-2.07723	-1.85677
F	2.27968	-4.55120	-5.06020
F	0.21224	-5.46050	-3.44435
C	0.94448	-4.36452	-3.07646
F	-0.48920	-3.96756	-1.21802
C	3.54518	-2.89037	-3.02770

```
F          4.31314       -1.83020       -2.68610
C          2.06854       -2.57533       -0.97436
F          2.81235       -1.51301       -0.57563
F          4.35748       -3.74719       -3.70234
C          2.12524       -4.82032       -2.16335
C          2.97688       -3.58046       -1.74901
F          1.60983       -3.16773        0.15282
F          2.90083       -5.72453       -2.81902
F          1.65199       -5.45574       -1.06548
F          4.01616       -3.98695       -0.95785
Al        -0.06556        0.05167       -0.00828

SCF energy GEOOPT =  -8053.020604483 H
ZPE =   1155. kJ/mol
FREEH energy =  1389.24 kJ/mol
FREEH entropy =   1.84778 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
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     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a               5.30         0.00857       YES     YES
     8        a              13.18         0.00849       YES     YES
     9        a              15.28         0.00649       YES     YES
    10        a              17.55         0.00585       YES     YES
    11        a              18.06         0.01841       YES     YES
    12        a              21.42         0.01732       YES     YES
    13        a              23.50         0.01168       YES     YES
    14        a              25.49         0.08732       YES     YES
    15        a              26.71         0.05698       YES     YES
    16        a              29.41         0.02276       YES     YES
    17        a              43.51         0.09529       YES     YES
    18        a              48.99         0.01086       YES     YES
    19        a              54.45         0.00734       YES     YES
    20        a              56.22         0.12313       YES     YES
    21        a              64.14         0.81890       YES     YES
    22        a              67.73         0.72480       YES     YES
    23        a              67.94         0.68305       YES     YES
    24        a              87.42         0.00176       YES     YES
    25        a             131.91         0.01770       YES     YES
    26        a             132.81         0.03412       YES     YES
    27        a             133.85         0.02652       YES     YES
    28        a             134.35         0.01910       YES     YES
    29        a             135.34         0.00904       YES     YES
    30        a             136.65         0.04992       YES     YES
    31        a             138.83         0.04518       YES     YES
    32        a             139.70         0.04930       YES     YES
    33        a             141.07         0.47522       YES     YES
    34        a             142.47         0.46468       YES     YES
    35        a             144.23         0.70979       YES     YES
    36        a             145.45         0.00613       YES     YES
    37        a             193.58         0.54402       YES     YES
    38        a             194.17         0.58533       YES     YES
    39        a             194.99         0.40028       YES     YES
    40        a             195.14         0.25057       YES     YES
    41        a             195.68         0.44444       YES     YES
    42        a             196.67         0.20435       YES     YES
    43        a             197.32         0.12337       YES     YES
    44        a             198.20         0.22555       YES     YES
    45        a             198.89         0.14128       YES     YES
    46        a             199.46         0.00898       YES     YES
    47        a             200.29         0.40895       YES     YES
    48        a             201.49         0.05353       YES     YES
    49        a             202.53         0.01813       YES     YES
    50        a             202.86         0.11361       YES     YES
```

51	a	203.08	0.08513	YES	YES
52	a	204.76	0.08131	YES	YES
53	a	205.02	0.05583	YES	YES
54	a	205.83	0.06592	YES	YES
55	a	206.16	0.05557	YES	YES
56	a	207.97	0.01457	YES	YES
57	a	224.55	0.01272	YES	YES
58	a	225.68	0.00245	YES	YES
59	a	225.98	0.00701	YES	YES
60	a	226.26	0.00620	YES	YES
61	a	242.01	0.28829	YES	YES
62	a	242.43	0.11890	YES	YES
63	a	243.03	0.47879	YES	YES
64	a	243.32	0.06885	YES	YES
65	a	243.82	0.19411	YES	YES
66	a	244.40	0.65296	YES	YES
67	a	244.68	0.47117	YES	YES
68	a	244.99	0.79458	YES	YES
69	a	245.28	0.07984	YES	YES
70	a	245.34	0.13137	YES	YES
71	a	245.55	0.23401	YES	YES
72	a	245.93	0.00339	YES	YES
73	a	246.02	0.11936	YES	YES
74	a	246.32	0.17186	YES	YES
75	a	246.42	0.35390	YES	YES
76	a	246.70	0.09506	YES	YES
77	a	247.11	0.01604	YES	YES
78	a	247.25	0.08933	YES	YES
79	a	247.35	0.13230	YES	YES
80	a	247.79	0.02719	YES	YES
81	a	251.65	2.95341	YES	YES
82	a	251.88	3.03135	YES	YES
83	a	253.14	2.72476	YES	YES
84	a	254.09	1.60029	YES	YES
85	a	255.25	0.74959	YES	YES
86	a	255.95	0.78458	YES	YES
87	a	256.78	0.12548	YES	YES
88	a	257.74	0.86187	YES	YES
89	a	258.53	0.32575	YES	YES
90	a	259.56	0.45898	YES	YES
91	a	260.06	0.27802	YES	YES
92	a	260.78	0.29679	YES	YES
93	a	262.56	0.01345	YES	YES
94	a	263.22	0.14721	YES	YES
95	a	263.44	0.15116	YES	YES
96	a	264.06	0.10876	YES	YES
97	a	268.36	0.40989	YES	YES
98	a	271.07	0.72710	YES	YES
99	a	273.52	5.42001	YES	YES
100	a	278.56	16.21236	YES	YES
101	a	281.48	19.91309	YES	YES
102	a	288.59	1.05850	YES	YES
103	a	293.84	11.28564	YES	YES
104	a	294.32	1.87011	YES	YES
105	a	296.25	3.82410	YES	YES
106	a	296.34	3.75326	YES	YES
107	a	296.79	13.89412	YES	YES
108	a	297.04	3.35519	YES	YES
109	a	297.53	1.64189	YES	YES
110	a	297.69	3.00446	YES	YES
111	a	297.90	0.44900	YES	YES
112	a	298.20	5.86066	YES	YES
113	a	298.40	6.57921	YES	YES
114	a	299.23	4.69267	YES	YES
115	a	299.66	9.24323	YES	YES
116	a	301.08	1.60563	YES	YES
117	a	301.50	2.23178	YES	YES
118	a	302.94	8.69576	YES	YES
119	a	306.12	0.19355	YES	YES
120	a	311.15	1.92554	YES	YES

121	a	312.22	2.87202	YES	YES
122	a	314.86	1.07872	YES	YES
123	a	330.78	6.08500	YES	YES
124	a	342.00	22.60759	YES	YES
125	a	361.73	1.21651	YES	YES
126	a	361.97	0.36482	YES	YES
127	a	363.35	1.15521	YES	YES
128	a	364.03	1.10519	YES	YES
129	a	373.08	23.03263	YES	YES
130	a	375.46	0.17202	YES	YES
131	a	376.26	0.17986	YES	YES
132	a	376.62	0.22927	YES	YES
133	a	377.06	0.58550	YES	YES
134	a	377.10	3.36361	YES	YES
135	a	377.43	2.91402	YES	YES
136	a	377.51	1.51204	YES	YES
137	a	378.00	0.27657	YES	YES
138	a	378.27	1.58486	YES	YES
139	a	378.41	0.45084	YES	YES
140	a	378.79	4.47651	YES	YES
141	a	380.06	0.03873	YES	YES
142	a	380.60	1.82742	YES	YES
143	a	380.98	3.34687	YES	YES
144	a	385.97	0.84952	YES	YES
145	a	386.67	1.15321	YES	YES
146	a	387.04	1.00241	YES	YES
147	a	388.11	0.84759	YES	YES
148	a	389.84	32.72750	YES	YES
149	a	391.15	7.77285	YES	YES
150	a	395.76	31.87443	YES	YES
151	a	399.56	45.55188	YES	YES
152	a	428.79	1.17770	YES	YES
153	a	429.88	5.51217	YES	YES
154	a	430.23	6.42144	YES	YES
155	a	430.30	12.20889	YES	YES
156	a	431.54	4.79153	YES	YES
157	a	432.05	0.18597	YES	YES
158	a	432.69	0.93237	YES	YES
159	a	432.73	14.38009	YES	YES
160	a	433.70	29.70940	YES	YES
161	a	434.03	28.25813	YES	YES
162	a	435.26	6.71077	YES	YES
163	a	436.19	43.20621	YES	YES
164	a	491.17	0.13446	YES	YES
165	a	522.69	13.23790	YES	YES
166	a	524.42	19.33356	YES	YES
167	a	526.58	22.74444	YES	YES
168	a	587.68	0.13683	YES	YES
169	a	588.43	0.11431	YES	YES
170	a	589.36	0.01905	YES	YES
171	a	589.72	0.01650	YES	YES
172	a	589.81	0.10057	YES	YES
173	a	590.00	0.04854	YES	YES
174	a	590.14	0.00476	YES	YES
175	a	590.48	0.16119	YES	YES
176	a	613.39	0.10751	YES	YES
177	a	628.04	19.78546	YES	YES
178	a	628.61	8.49965	YES	YES
179	a	629.09	15.77919	YES	YES
180	a	634.64	2.17967	YES	YES
181	a	634.90	15.12259	YES	YES
182	a	635.05	2.75888	YES	YES
183	a	635.35	5.88339	YES	YES
184	a	635.61	9.37901	YES	YES
185	a	635.67	9.22558	YES	YES
186	a	635.99	21.49282	YES	YES
187	a	636.04	21.77032	YES	YES
188	a	649.94	0.00802	YES	YES
189	a	666.32	18.03496	YES	YES
190	a	666.81	18.15553	YES	YES

191	a	667.78	18.61114	YES	YES
192	a	709.31	0.07833	YES	YES
193	a	754.79	21.11263	YES	YES
194	a	755.92	25.94393	YES	YES
195	a	761.40	25.41891	YES	YES
196	a	833.49	0.03849	YES	YES
197	a	833.61	0.02610	YES	YES
198	a	833.78	0.02746	YES	YES
199	a	833.89	0.09249	YES	YES
200	a	834.29	0.03550	YES	YES
201	a	834.65	0.01445	YES	YES
202	a	835.31	0.01334	YES	YES
203	a	835.67	0.01761	YES	YES
204	a	836.39	0.25387	YES	YES
205	a	836.54	0.34630	YES	YES
206	a	837.27	0.17420	YES	YES
207	a	837.91	0.48901	YES	YES
208	a	952.08	12.62124	YES	YES
209	a	952.25	22.38682	YES	YES
210	a	954.59	0.32556	YES	YES
211	a	957.28	25.32788	YES	YES
212	a	958.99	120.87394	YES	YES
213	a	960.06	677.03663	YES	YES
214	a	960.98	604.18892	YES	YES
215	a	961.76	622.85108	YES	YES
216	a	971.42	483.50705	YES	YES
217	a	972.50	557.44559	YES	YES
218	a	973.00	455.73474	YES	YES
219	a	978.48	10.31846	YES	YES
220	a	980.09	17.67636	YES	YES
221	a	980.98	11.90079	YES	YES
222	a	981.22	19.62927	YES	YES
223	a	982.39	26.05817	YES	YES
224	a	983.60	11.39895	YES	YES
225	a	983.98	16.40703	YES	YES
226	a	984.25	7.59072	YES	YES
227	a	985.01	9.36707	YES	YES
228	a	1023.97	3.13172	YES	YES
229	a	1025.66	1.56216	YES	YES
230	a	1026.40	5.90379	YES	YES
231	a	1027.29	1.46824	YES	YES
232	a	1028.45	3.02654	YES	YES
233	a	1028.98	3.68622	YES	YES
234	a	1029.24	3.93898	YES	YES
235	a	1029.64	0.93637	YES	YES
236	a	1054.34	1.04649	YES	YES
237	a	1054.70	0.61039	YES	YES
238	a	1054.83	1.03624	YES	YES
239	a	1055.20	1.70961	YES	YES
240	a	1055.25	1.05000	YES	YES
241	a	1055.86	1.16852	YES	YES
242	a	1056.55	1.56171	YES	YES
243	a	1056.78	1.28915	YES	YES
244	a	1065.49	0.14238	YES	YES
245	a	1066.80	0.49174	YES	YES
246	a	1067.53	0.90970	YES	YES
247	a	1068.72	1.39689	YES	YES
248	a	1093.89	75.07778	YES	YES
249	a	1094.15	75.59647	YES	YES
250	a	1095.83	66.20348	YES	YES
251	a	1098.43	11.90116	YES	YES
252	a	1118.08	0.54222	YES	YES
253	a	1120.09	0.23967	YES	YES
254	a	1120.62	1.32921	YES	YES
255	a	1121.01	1.53059	YES	YES
256	a	1121.29	0.30981	YES	YES
257	a	1121.83	0.07471	YES	YES
258	a	1122.46	1.30074	YES	YES
259	a	1122.95	0.86454	YES	YES
260	a	1127.73	0.37708	YES	YES

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   261        a            1129.73         0.03036       YES     YES
   262        a            1130.77         0.19507       YES     YES
   263        a            1131.38         0.39070       YES     YES
   264        a            1196.74         1.19235       YES     YES
   265        a            1197.23         0.98608       YES     YES
   266        a            1197.95         1.28703       YES     YES
   267        a            1199.47         1.22875       YES     YES
   268        a            1199.63         0.81908       YES     YES
   269        a            1201.02         1.25699       YES     YES
   270        a            1204.11         6.45103       YES     YES
   271        a            1204.89         7.51398       YES     YES
   272        a            1205.33         4.75641       YES     YES
   273        a            1205.98        14.85737       YES     YES
   274        a            1206.85         7.41428       YES     YES
   275        a            1207.44        12.84919       YES     YES
   276        a            1208.15         8.70215       YES     YES
   277        a            1208.73        17.83247       YES     YES
   278        a            1209.61        11.93751       YES     YES
   279        a            1209.94         8.88545       YES     YES
   280        a            1210.97         5.58837       YES     YES
   281        a            1211.30         1.96317       YES     YES
   282        a            1212.07         5.85669       YES     YES
   283        a            1212.38         6.43084       YES     YES
   284        a            1232.18        22.01544       YES     YES
   285        a            1233.00        28.32506       YES     YES
   286        a            1233.67        13.76259       YES     YES
   287        a            1235.27         0.71646       YES     YES
   288        a            1244.47        13.82120       YES     YES
   289        a            1246.62         7.09867       YES     YES
   290        a            1248.52       947.33431       YES     YES
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   292        a            1250.27       897.88754       YES     YES
   293        a            1252.02       143.60806       YES     YES
   294        a            1252.99         9.89387       YES     YES
   295        a            1253.19        77.82361       YES     YES
   296        a            1254.12        50.46925       YES     YES
   297        a            1254.47        17.67420       YES     YES
   298        a            1255.01        20.21579       YES     YES
   299        a            1255.41        86.92773       YES     YES
   300        a            1255.68        40.51590       YES     YES
   301        a            1256.60        90.05856       YES     YES
   302        a            1256.85       117.87336       YES     YES
   303        a            1257.40       245.84351       YES     YES
   304        a            1259.91       518.37604       YES     YES
   305        a            1261.46       542.76806       YES     YES
   306        a            1261.51        47.20083       YES     YES
   307        a            1263.13       315.83141       YES     YES
   308        a            1280.08       146.22366       YES     YES
   309        a            1280.59       159.79486       YES     YES
   310        a            1280.95       166.05942       YES     YES
   311        a            1288.76         0.91626       YES     YES
   312        a            1361.67       438.38318       YES     YES
   313        a            1363.43       468.03061       YES     YES
   314        a            1368.14       457.02983       YES     YES
   315        a            1398.84        13.78319       YES     YES
$end
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$Al(OC_{10}F_{15})_3 \cdot OC_{10}F_{14}$ (1)

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C         -2.36118       -0.70045       -1.70773
C         -2.60442       -2.07258       -2.42438
C         -2.14052        0.38113       -2.82200
C         -3.67142       -0.32826       -0.91541
C         -3.58424       -0.89299       -4.46788
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C	-3.83498	-1.99013	-3.38472
C	-5.11179	-1.62081	-2.56233
C	-4.90332	-0.23785	-1.86515
C	-4.64210	0.86014	-2.94580
C	-3.36817	0.49315	-3.77179
F	-3.90145	-1.25081	0.04817
F	-3.49965	0.85762	-0.28068
F	-2.81414	-3.04818	-1.50866
F	-1.88467	1.57994	-2.21351
F	-1.03509	0.08953	-3.54262
F	-4.63609	-0.82515	-5.31703
F	-2.50381	-1.21609	-5.21500
F	-3.14679	1.44882	-4.71720
F	-5.71337	0.96989	-3.76575
F	-4.47440	2.06729	-2.35788
F	-6.01873	0.08474	-1.14996
F	-5.35969	-2.57622	-1.63684
F	-6.19453	-1.57806	-3.37350
F	-4.01944	-3.19690	-3.99352
F	-1.50205	-2.43329	-3.12706
O	-1.28864	-0.78421	-0.86844
Al	-0.21561	0.39975	-0.16516
C	0.45709	-1.53157	2.12399
C	2.31424	0.51630	-1.66080
C	-0.73761	2.61253	1.71193
C	1.73008	-1.99541	2.87748
C	2.54819	1.18795	-3.06657
C	-0.86540	2.05163	3.17299
C	-0.89934	-2.01018	2.70390
C	2.38938	-1.03667	-1.86579
C	0.67426	3.28794	1.57225
C	0.66721	-4.21545	-0.34610
C	3.50732	0.94839	-0.72422
C	-1.82967	3.72836	1.52392
C	0.35214	-3.87222	3.93278
C	3.95614	-0.80299	-3.83977
C	0.73474	3.81284	4.06611
C	1.68672	-3.52873	3.19845
C	3.92678	0.75087	-3.66941
C	-0.68064	3.17080	4.23584
C	1.79601	-4.37876	1.88788
C	5.08133	1.18344	-2.70871
C	-1.77705	4.26235	4.01891
C	0.56511	-4.19682	1.01515
C	4.88315	0.50795	-1.31328
C	-1.64631	4.86496	2.58199
C	-0.78207	-4.38075	1.69931
C	4.90250	-1.04535	-1.47951
C	-0.23008	5.50641	2.42048
C	-0.87267	-3.54419	3.01704
C	3.75708	-1.48503	-2.44775
C	0.86974	4.41581	2.63006
F	1.79098	-4.28689	-1.00053
F	3.49456	2.28776	-0.54876
F	-3.06460	3.18955	1.64414
F	-0.34490	-4.18194	-1.16056
F	3.34112	0.39489	0.50474
F	-1.74669	4.24340	0.27496
F	2.81944	-1.67350	2.16846
F	2.50633	2.53364	-2.94890
F	-2.06067	1.44270	3.33328
F	-1.89093	-1.68198	1.86247
F	2.18183	-1.65686	-0.65960
F	0.82981	3.78926	0.32731
F	-1.09247	-1.33905	3.87020
F	1.37964	-1.45889	-2.66188
F	1.63882	2.33921	1.72944
F	0.33291	-5.18356	4.25949
F	5.13251	-1.19716	-4.38069
F	0.92198	4.77474	4.99818

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F          0.27095       -3.17607        5.09100
F          2.98372       -1.20152       -4.69233
F          1.69685        2.88246        4.27154
F         -2.02058       -3.85924        3.67934
F          3.77981       -2.84228       -2.59445
F          2.10340        4.97812        2.48770
F         -0.95930       -5.69557        2.02221
F          6.09786       -1.45489       -1.96049
F         -0.06604        6.50672        3.31815
F         -1.81522       -4.03434        0.89477
F          4.74452       -1.64585       -0.27457
F         -0.10565        6.06107        1.19332
F          5.89205        0.88601       -0.47700
F         -2.60104        5.82143        2.40409
F          2.93429       -4.03194        1.23563
F          5.09863        2.52903       -2.57811
F         -3.00612        3.72239        4.18905
F          1.93409       -5.68834        2.24610
F          6.28122        0.82761       -3.22757
F         -1.64840        5.23674        4.94950
F          4.10338        1.34051       -4.88606
F         -0.79840        2.64726        5.48996
F          1.75787       -1.29399        4.04367
F          1.55614        0.83876       -3.91885
F          0.08157        1.08362        3.36913
O          0.55367       -0.73917        1.19702
O          1.12962        0.90316       -1.13147
O         -0.93375        1.61935        0.81523
F          2.73706       -3.82079        4.01505

SCF energy GEOOPT =  -7953.039629421 H
ZPE =   1146. kJ/mol
FREEH energy =  1380.79 kJ/mol
FREEH entropy =   1.85096 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000         -       -
     2                      -0.00         0.00000         -       -
     3                      -0.00         0.00000         -       -
     4                      -0.00         0.00000         -       -
     5                       0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
     7        a             12.92         0.03184       YES     YES
     8        a             13.87         0.02263       YES     YES
     9        a             17.20         0.00902       YES     YES
    10        a             18.04         0.04320       YES     YES
    11        a             20.20         0.08270       YES     YES
    12        a             23.42         0.04792       YES     YES
    13        a             26.20         0.12572       YES     YES
    14        a             29.42         0.04593       YES     YES
    15        a             31.06         0.17357       YES     YES
    16        a             33.24         0.44759       YES     YES
    17        a             36.48         0.17714       YES     YES
    18        a             41.67         0.13759       YES     YES
    19        a             45.24         0.50463       YES     YES
    20        a             48.83         0.30043       YES     YES
    21        a             58.76         0.82014       YES     YES
    22        a             61.14         0.55590       YES     YES
    23        a             63.27         1.19554       YES     YES
    24        a             73.46         0.32081       YES     YES
    25        a             80.66         0.86192       YES     YES
    26        a             93.26         0.50846       YES     YES
    27        a            119.66         0.24821       YES     YES
    28        a            130.42         1.00462       YES     YES
    29        a            133.14         0.15644       YES     YES
    30        a            134.87         0.13194       YES     YES
    31        a            135.23         0.03641       YES     YES
    32        a            135.90         0.41428       YES     YES
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33	a	138.39	0.06015	YES	YES
34	a	139.91	0.22335	YES	YES
35	a	142.21	0.74277	YES	YES
36	a	143.09	0.44785	YES	YES
37	a	146.24	0.45287	YES	YES
38	a	152.03	1.57208	YES	YES
39	a	158.04	0.23992	YES	YES
40	a	175.17	0.38578	YES	YES
41	a	180.25	2.45676	YES	YES
42	a	185.19	6.06922	YES	YES
43	a	193.61	0.73615	YES	YES
44	a	193.74	0.77804	YES	YES
45	a	195.89	0.17579	YES	YES
46	a	196.87	0.12926	YES	YES
47	a	197.50	0.52191	YES	YES
48	a	198.12	0.06024	YES	YES
49	a	200.29	0.61718	YES	YES
50	a	201.31	0.09594	YES	YES
51	a	201.47	0.17940	YES	YES
52	a	202.07	1.00165	YES	YES
53	a	203.40	0.22201	YES	YES
54	a	203.63	0.14947	YES	YES
55	a	204.89	0.08310	YES	YES
56	a	205.16	0.13852	YES	YES
57	a	206.43	0.11144	YES	YES
58	a	207.52	1.07130	YES	YES
59	a	223.90	0.50876	YES	YES
60	a	225.83	0.80391	YES	YES
61	a	226.56	0.09423	YES	YES
62	a	228.68	0.86722	YES	YES
63	a	233.05	0.18426	YES	YES
64	a	241.95	8.92282	YES	YES
65	a	243.32	0.99498	YES	YES
66	a	243.44	0.59704	YES	YES
67	a	244.30	2.70942	YES	YES
68	a	244.36	0.35205	YES	YES
69	a	244.69	0.36748	YES	YES
70	a	245.27	0.42689	YES	YES
71	a	245.80	0.14610	YES	YES
72	a	246.13	0.08434	YES	YES
73	a	246.30	0.61602	YES	YES
74	a	246.49	0.00358	YES	YES
75	a	246.89	0.25699	YES	YES
76	a	247.39	0.72561	YES	YES
77	a	247.63	0.55334	YES	YES
78	a	248.30	0.32073	YES	YES
79	a	249.68	0.32374	YES	YES
80	a	251.20	1.71740	YES	YES
81	a	252.02	1.33381	YES	YES
82	a	253.35	1.91587	YES	YES
83	a	253.61	1.11752	YES	YES
84	a	255.05	2.30970	YES	YES
85	a	255.71	11.72317	YES	YES
86	a	255.94	0.68717	YES	YES
87	a	258.04	1.89285	YES	YES
88	a	258.19	1.75988	YES	YES
89	a	259.03	2.45420	YES	YES
90	a	260.10	0.27474	YES	YES
91	a	260.77	2.59394	YES	YES
92	a	261.75	5.14767	YES	YES
93	a	262.03	3.52567	YES	YES
94	a	263.65	0.21788	YES	YES
95	a	264.68	1.75258	YES	YES
96	a	268.72	1.43697	YES	YES
97	a	274.09	0.18302	YES	YES
98	a	275.12	17.23551	YES	YES
99	a	278.81	8.34433	YES	YES
100	a	282.72	1.22283	YES	YES
101	a	287.58	8.92771	YES	YES
102	a	288.26	3.91842	YES	YES

103	a	289.77	6.00351	YES	YES
104	a	294.84	2.50840	YES	YES
105	a	295.37	9.84543	YES	YES
106	a	296.89	4.42574	YES	YES
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108	a	297.77	2.54661	YES	YES
109	a	298.31	9.19740	YES	YES
110	a	298.35	3.27226	YES	YES
111	a	298.96	7.23667	YES	YES
112	a	299.26	5.65131	YES	YES
113	a	299.79	2.32616	YES	YES
114	a	302.47	2.31467	YES	YES
115	a	304.14	2.60412	YES	YES
116	a	306.72	5.06241	YES	YES
117	a	308.36	1.98363	YES	YES
118	a	311.69	2.37370	YES	YES
119	a	312.76	0.33725	YES	YES
120	a	317.29	1.46421	YES	YES
121	a	327.25	2.19546	YES	YES
122	a	334.55	1.62693	YES	YES
123	a	340.39	36.22029	YES	YES
124	a	351.73	6.73799	YES	YES
125	a	358.60	5.47358	YES	YES
126	a	362.80	0.05395	YES	YES
127	a	364.59	0.39478	YES	YES
128	a	365.34	0.26805	YES	YES
129	a	367.45	4.72526	YES	YES
130	a	370.90	5.05923	YES	YES
131	a	375.94	14.30568	YES	YES
132	a	377.00	0.38369	YES	YES
133	a	378.23	0.33873	YES	YES
134	a	378.40	0.19947	YES	YES
135	a	378.92	1.10466	YES	YES
136	a	379.05	0.73630	YES	YES
137	a	379.82	0.31465	YES	YES
138	a	379.98	0.17089	YES	YES
139	a	380.13	1.81600	YES	YES
140	a	380.47	0.60905	YES	YES
141	a	381.85	4.81269	YES	YES
142	a	385.55	3.17733	YES	YES
143	a	387.85	3.98033	YES	YES
144	a	388.92	1.12057	YES	YES
145	a	389.82	11.57432	YES	YES
146	a	391.46	11.55002	YES	YES
147	a	393.84	23.00953	YES	YES
148	a	398.90	2.58766	YES	YES
149	a	405.31	20.13721	YES	YES
150	a	410.74	3.61480	YES	YES
151	a	416.86	16.06707	YES	YES
152	a	428.77	5.46085	YES	YES
153	a	430.50	10.79621	YES	YES
154	a	431.62	11.67499	YES	YES
155	a	432.31	9.02376	YES	YES
156	a	433.93	7.72539	YES	YES
157	a	434.28	6.89988	YES	YES
158	a	434.64	9.41322	YES	YES
159	a	435.03	24.84043	YES	YES
160	a	435.93	19.74872	YES	YES
161	a	439.36	14.43808	YES	YES
162	a	500.16	3.23201	YES	YES
163	a	529.79	7.37537	YES	YES
164	a	532.01	7.48171	YES	YES
165	a	537.47	13.19645	YES	YES
166	a	564.36	23.67312	YES	YES
167	a	572.01	3.57818	YES	YES
168	a	588.94	0.02968	YES	YES
169	a	589.24	0.02722	YES	YES
170	a	589.49	0.19377	YES	YES
171	a	590.29	0.02504	YES	YES
172	a	590.55	0.03604	YES	YES

173	a	590.95	0.12654	YES	YES
174	a	600.07	14.44299	YES	YES
175	a	604.94	9.85840	YES	YES
176	a	620.38	4.03811	YES	YES
177	a	629.41	7.26603	YES	YES
178	a	631.52	14.60583	YES	YES
179	a	632.38	16.92704	YES	YES
180	a	633.59	12.02945	YES	YES
181	a	634.94	5.77847	YES	YES
182	a	635.57	6.90103	YES	YES
183	a	635.77	4.68890	YES	YES
184	a	636.42	24.62136	YES	YES
185	a	636.57	9.38899	YES	YES
186	a	637.26	22.63984	YES	YES
187	a	653.77	3.53620	YES	YES
188	a	664.08	10.88466	YES	YES
189	a	672.18	11.85823	YES	YES
190	a	673.76	12.61036	YES	YES
191	a	718.21	1.55185	YES	YES
192	a	728.71	44.91970	YES	YES
193	a	737.22	3.33216	YES	YES
194	a	794.15	24.28001	YES	YES
195	a	805.14	6.06399	YES	YES
196	a	818.78	0.54724	YES	YES
197	a	832.22	0.57304	YES	YES
198	a	832.92	0.12332	YES	YES
199	a	834.99	0.19610	YES	YES
200	a	835.41	0.03688	YES	YES
201	a	835.90	0.10621	YES	YES
202	a	836.33	0.71864	YES	YES
203	a	837.50	0.08043	YES	YES
204	a	838.07	0.09366	YES	YES
205	a	838.64	0.30801	YES	YES
206	a	842.53	0.58266	YES	YES
207	a	894.83	146.64209	YES	YES
208	a	950.34	90.55934	YES	YES
209	a	955.12	26.68653	YES	YES
210	a	956.46	110.62537	YES	YES
211	a	958.21	258.87767	YES	YES
212	a	961.49	222.79440	YES	YES
213	a	961.80	431.58952	YES	YES
214	a	963.57	632.03023	YES	YES
215	a	975.58	549.54850	YES	YES
216	a	977.18	363.92267	YES	YES
217	a	979.60	343.31461	YES	YES
218	a	983.09	99.20450	YES	YES
219	a	983.81	20.60021	YES	YES
220	a	985.61	14.87534	YES	YES
221	a	985.96	20.20281	YES	YES
222	a	986.33	17.66723	YES	YES
223	a	989.33	7.72703	YES	YES
224	a	991.83	1.68339	YES	YES
225	a	993.96	0.76507	YES	YES
226	a	1010.11	36.48753	YES	YES
227	a	1032.82	4.72230	YES	YES
228	a	1040.67	8.84687	YES	YES
229	a	1042.24	6.95129	YES	YES
230	a	1042.65	5.01078	YES	YES
231	a	1045.76	6.83280	YES	YES
232	a	1048.34	5.91627	YES	YES
233	a	1051.99	1.95577	YES	YES
234	a	1053.02	1.98557	YES	YES
235	a	1054.13	1.00175	YES	YES
236	a	1055.46	0.40216	YES	YES
237	a	1056.73	1.37411	YES	YES
238	a	1057.55	0.45535	YES	YES
239	a	1059.45	6.09363	YES	YES
240	a	1059.82	1.40618	YES	YES
241	a	1060.76	0.28937	YES	YES
242	a	1061.74	2.34386	YES	YES

243	a	1065.20	16.91224	YES	YES
244	a	1074.04	22.50234	YES	YES
245	a	1088.83	0.41754	YES	YES
246	a	1094.42	71.54385	YES	YES
247	a	1095.85	34.52242	YES	YES
248	a	1102.26	48.25439	YES	YES
249	a	1109.32	57.41743	YES	YES
250	a	1110.38	27.63692	YES	YES
251	a	1118.28	1.73221	YES	YES
252	a	1118.92	12.31989	YES	YES
253	a	1127.18	6.44109	YES	YES
254	a	1128.98	2.62121	YES	YES
255	a	1129.56	1.43861	YES	YES
256	a	1130.26	1.29381	YES	YES
257	a	1131.86	3.28949	YES	YES
258	a	1132.12	0.92016	YES	YES
259	a	1133.79	0.43041	YES	YES
260	a	1141.53	1.21024	YES	YES
261	a	1154.04	109.96613	YES	YES
262	a	1195.46	1.83630	YES	YES
263	a	1196.34	23.92798	YES	YES
264	a	1198.25	18.20664	YES	YES
265	a	1200.31	10.51585	YES	YES
266	a	1204.41	24.33312	YES	YES
267	a	1205.17	1.82222	YES	YES
268	a	1206.80	9.08491	YES	YES
269	a	1209.08	0.10461	YES	YES
270	a	1209.56	29.54632	YES	YES
271	a	1210.03	15.69206	YES	YES
272	a	1211.17	17.60158	YES	YES
273	a	1211.46	10.07637	YES	YES
274	a	1211.93	11.36652	YES	YES
275	a	1212.46	22.49436	YES	YES
276	a	1213.78	21.91762	YES	YES
277	a	1214.23	7.25763	YES	YES
278	a	1215.62	5.73730	YES	YES
279	a	1225.55	79.13673	YES	YES
280	a	1232.62	145.28913	YES	YES
281	a	1233.09	258.37602	YES	YES
282	a	1237.95	28.19315	YES	YES
283	a	1238.31	75.38013	YES	YES
284	a	1241.24	169.88386	YES	YES
285	a	1242.81	65.27865	YES	YES
286	a	1248.75	276.89610	YES	YES
287	a	1250.07	144.24412	YES	YES
288	a	1252.41	494.75805	YES	YES
289	a	1255.96	128.21620	YES	YES
290	a	1256.58	265.66590	YES	YES
291	a	1258.59	106.33940	YES	YES
292	a	1260.30	275.62108	YES	YES
293	a	1260.42	215.44204	YES	YES
294	a	1261.10	298.45062	YES	YES
295	a	1261.63	290.74232	YES	YES
296	a	1262.10	181.32997	YES	YES
297	a	1262.79	361.39679	YES	YES
298	a	1263.36	55.75088	YES	YES
299	a	1264.35	406.01600	YES	YES
300	a	1265.45	167.40633	YES	YES
301	a	1266.47	53.80533	YES	YES
302	a	1278.51	91.36141	YES	YES
303	a	1279.89	164.54927	YES	YES
304	a	1282.86	157.51847	YES	YES
305	a	1284.36	86.48324	YES	YES
306	a	1290.37	41.80584	YES	YES
307	a	1327.41	157.69576	YES	YES
308	a	1352.09	298.27858	YES	YES
309	a	1368.11	163.56642	YES	YES
310	a	1392.45	408.25969	YES	YES
311	a	1674.25	539.28105	YES	YES
312	a	1764.22	261.85972	YES	YES

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$end
```

$Al(OC_{10}F_{15})_3 \cdot OC_{10}F_{14}$ (2, epoxid)

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Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C         -1.61453       -3.50748       -3.97604
C         -0.76880       -4.74326       -3.52901
C          0.64065       -4.27122       -3.04965
C          1.37150       -3.53335       -4.21875
C          0.53025       -2.29497       -4.66648
C         -0.88079       -2.77407       -5.14564
C          0.34992       -1.32075       -3.46139
C          0.46878       -3.28670       -1.85460
C         -1.77654       -2.52546       -2.77249
C         -0.37749       -2.02982       -2.26520
F         -1.40256       -5.40069       -2.52978
F         -0.64388       -5.62036       -4.55240
F          1.37717       -5.35195       -2.66494
F          1.54927       -4.37953       -5.26031
F          2.60348       -3.13648       -3.82501
F          1.16640       -1.65737       -5.68926
F         -1.61547       -1.71725       -5.56379
F         -0.75490       -3.60375       -6.20763
F         -2.84112       -3.92560       -4.40039
F         -0.35481       -0.23551       -3.85421
F          1.55787       -0.85698       -3.03919
F         -0.12126       -3.91424       -0.80947
F          1.68761       -2.87909       -1.42360
F         -2.53965       -1.46943       -3.14151
F         -2.43764       -3.14111       -1.76041
O         -0.55031       -1.18881       -1.21337
Al         0.23962       -0.11830       -0.10992
C          3.85883       -0.17065        3.71917
C          4.95143        0.35040        2.73328
C          4.93620       -0.51416        1.43143
C          5.22420       -2.00672        1.79144
C          4.13291       -2.52832        2.78112
C          4.15758       -1.66261        4.08011
C          2.72570       -2.42106        2.10647
C          3.53132       -0.41037        0.76792
C          2.45256       -0.07821        3.04325
C          2.39609       -0.93002        1.72174
F          4.72186        1.65068        2.43549
F          6.17371        0.29374        3.31234
F          5.88855       -0.05741        0.56927
F          6.45304       -2.12470        2.34683
F          5.23324       -2.76024        0.66786
F          4.39320       -3.82936        3.09654
F          3.24382       -2.12471        4.96452
F          5.36481       -1.76290        4.68596
F          3.87182        0.58556        4.85381
F          1.77697       -2.90075        2.94594
F          2.69923       -3.20520        1.00563
F          3.28541        0.88018        0.42568
F          3.51056       -1.11428       -0.39168
F          1.51407       -0.50772        3.92025
F          2.15460        1.21568        2.76447
O          1.16640       -0.86032        1.14115
O          0.66482        1.47317       -0.58863
F         -0.75811        2.26489       -2.88510
F         -1.98958        2.23550       -1.10175
F          2.62816        3.45572       -0.79780
F          1.77034        2.90344       -2.71657
F          1.13777        3.44230        1.34879
F         -0.95226        2.87619        1.22486
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F         -2.46664        4.43638       -2.72205
F         -2.64999        4.46759        0.05329
F         -1.98034        6.36049       -0.77384
F         -0.56844        5.61893        1.50220
F          1.95751        5.69872        0.34339
F          0.54081        7.02474       -0.62809
F          2.14965        5.64671       -2.43127
F          0.06100        4.51197       -3.88155
F         -0.48454        6.38368       -2.92754
C          0.32826        2.76428       -0.80641
C         -0.95362        2.88862       -1.70485
C          1.50048        3.51662       -1.54095
C          0.05720        3.51381        0.54743
C         -1.61409        5.07388       -0.58007
C         -0.33197        5.00342        0.30854
C          0.84776        5.72142       -0.42760
C          1.12328        5.01506       -1.79547
C         -0.16234        5.09250       -2.68049
C         -1.34458        4.37534       -1.95066
F         -4.27243        1.83203        0.23861
F         -3.29006       -0.33739       -0.59933
F         -3.83679        2.68401        2.18510
C         -3.87964        1.54358        1.48650
O         -1.57287        0.09658        0.73935
F         -5.57452       -0.60488        0.11962
C         -2.84043       -0.53281        0.64434
C         -2.63241        0.63048        1.58648
F         -6.17755        1.15550        2.12188
C         -4.97441        0.52405        2.15115
C         -5.09708       -0.84322        1.35549
C         -3.67669       -1.61377        1.32738
F         -2.11817        1.54891        3.73507
C         -2.19803        0.37693        3.06688
F         -3.80183       -2.78404        0.66444
F         -0.97095       -0.17345        3.09718
F         -5.99354       -1.65424        1.95589
F         -4.56395        1.29545        4.37682
C         -4.61493        0.16650        3.63370
C         -3.23879       -0.57651        3.68390
C         -3.24855       -1.88608        2.80911
F         -2.01429       -2.44857        2.79029
F         -5.57483       -0.61315        4.17982
F         -4.09497       -2.78076        3.35730
F         -2.93366       -0.89353        4.96970

SCF energy GEOOPT =  -7952.956663941 H
ZPE =   1146. kJ/mol
FREEH energy =  1377.70 kJ/mol
FREEH entropy =   1.82934 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000         -       -
     2                      -0.00         0.00000         -       -
     3                      -0.00         0.00000         -       -
     4                      -0.00         0.00000         -       -
     5                      -0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
     7        a              9.41         0.00908       YES     YES
     8        a             13.20         0.00080       YES     YES
     9        a             14.75         0.00874       YES     YES
    10        a             20.06         0.00299       YES     YES
    11        a             21.34         0.00025       YES     YES
    12        a             22.16         0.02938       YES     YES
    13        a             23.82         0.01141       YES     YES
    14        a             26.44         0.03036       YES     YES
    15        a             28.82         0.02758       YES     YES
    16        a             29.42         0.05309       YES     YES
    17        a             34.92         0.12438       YES     YES
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18	a	41.58	0.15706	YES	YES
19	a	48.23	0.09987	YES	YES
20	a	56.30	0.87932	YES	YES
21	a	64.14	0.60869	YES	YES
22	a	67.24	0.01722	YES	YES
23	a	68.19	2.03799	YES	YES
24	a	89.51	0.04578	YES	YES
25	a	114.85	0.06191	YES	YES
26	a	128.18	0.10411	YES	YES
27	a	131.39	0.00786	YES	YES
28	a	133.31	0.01724	YES	YES
29	a	133.76	0.00613	YES	YES
30	a	135.48	0.01505	YES	YES
31	a	136.01	0.06667	YES	YES
32	a	136.97	0.00661	YES	YES
33	a	140.33	0.38774	YES	YES
34	a	140.56	0.69217	YES	YES
35	a	144.41	0.26727	YES	YES
36	a	155.28	0.24003	YES	YES
37	a	186.29	1.23359	YES	YES
38	a	192.83	1.35796	YES	YES
39	a	193.72	0.91881	YES	YES
40	a	193.94	0.67647	YES	YES
41	a	194.68	0.42250	YES	YES
42	a	196.34	1.76658	YES	YES
43	a	196.80	0.94937	YES	YES
44	a	198.42	0.52592	YES	YES
45	a	199.32	0.40829	YES	YES
46	a	200.22	0.81923	YES	YES
47	a	201.43	0.29190	YES	YES
48	a	203.15	0.30791	YES	YES
49	a	203.32	0.02982	YES	YES
50	a	204.18	0.64200	YES	YES
51	a	205.10	0.00980	YES	YES
52	a	205.53	0.96885	YES	YES
53	a	206.08	0.22383	YES	YES
54	a	206.62	0.15481	YES	YES
55	a	217.28	5.57383	YES	YES
56	a	224.80	0.16108	YES	YES
57	a	224.94	0.02467	YES	YES
58	a	225.74	0.03965	YES	YES
59	a	226.10	0.10135	YES	YES
60	a	226.31	0.85155	YES	YES
61	a	235.11	7.65078	YES	YES
62	a	238.60	17.99124	YES	YES
63	a	240.27	10.95864	YES	YES
64	a	243.21	0.03268	YES	YES
65	a	243.44	0.20251	YES	YES
66	a	244.12	2.17053	YES	YES
67	a	244.71	0.17704	YES	YES
68	a	244.92	0.17509	YES	YES
69	a	245.48	2.11633	YES	YES
70	a	245.59	2.39690	YES	YES
71	a	245.64	0.00973	YES	YES
72	a	245.86	0.11960	YES	YES
73	a	246.06	0.37655	YES	YES
74	a	246.76	1.78407	YES	YES
75	a	246.97	0.11871	YES	YES
76	a	247.46	2.73698	YES	YES
77	a	247.71	0.58267	YES	YES
78	a	247.90	4.51162	YES	YES
79	a	248.51	2.58509	YES	YES
80	a	248.71	1.82985	YES	YES
81	a	251.80	3.81137	YES	YES
82	a	252.54	2.09527	YES	YES
83	a	253.35	0.26035	YES	YES
84	a	255.00	0.38910	YES	YES
85	a	255.41	1.65373	YES	YES
86	a	255.73	0.24767	YES	YES
87	a	256.78	0.84971	YES	YES

88	a	257.75	1.00166	YES	YES
89	a	258.32	3.48375	YES	YES
90	a	258.72	0.65330	YES	YES
91	a	259.01	0.65305	YES	YES
92	a	260.05	12.92998	YES	YES
93	a	262.78	0.06512	YES	YES
94	a	263.35	1.41354	YES	YES
95	a	263.71	0.05679	YES	YES
96	a	269.16	0.51127	YES	YES
97	a	272.36	0.31993	YES	YES
98	a	275.49	1.31926	YES	YES
99	a	277.16	30.60845	YES	YES
100	a	285.75	2.20263	YES	YES
101	a	288.54	2.26958	YES	YES
102	a	292.38	25.05340	YES	YES
103	a	293.35	3.94749	YES	YES
104	a	294.18	1.58670	YES	YES
105	a	296.00	5.56929	YES	YES
106	a	296.05	4.95546	YES	YES
107	a	297.30	3.72606	YES	YES
108	a	297.45	2.34413	YES	YES
109	a	298.13	8.54959	YES	YES
110	a	298.55	5.81437	YES	YES
111	a	298.97	8.10823	YES	YES
112	a	299.68	12.82020	YES	YES
113	a	300.12	4.02735	YES	YES
114	a	301.71	0.71595	YES	YES
115	a	305.63	5.66734	YES	YES
116	a	306.33	1.02051	YES	YES
117	a	310.04	1.35447	YES	YES
118	a	312.60	2.67802	YES	YES
119	a	314.97	3.47457	YES	YES
120	a	323.50	24.00110	YES	YES
121	a	323.71	10.50142	YES	YES
122	a	338.95	13.25495	YES	YES
123	a	343.77	7.49065	YES	YES
124	a	361.89	2.08693	YES	YES
125	a	362.50	0.08269	YES	YES
126	a	363.34	0.56578	YES	YES
127	a	365.14	2.29311	YES	YES
128	a	373.90	5.78292	YES	YES
129	a	375.05	15.79304	YES	YES
130	a	377.26	0.35510	YES	YES
131	a	377.75	0.71398	YES	YES
132	a	378.33	1.46889	YES	YES
133	a	378.70	0.13579	YES	YES
134	a	378.81	0.25236	YES	YES
135	a	379.33	0.65992	YES	YES
136	a	379.60	0.86732	YES	YES
137	a	380.06	1.08543	YES	YES
138	a	381.35	1.21971	YES	YES
139	a	382.47	0.82759	YES	YES
140	a	384.99	4.10824	YES	YES
141	a	387.67	2.33672	YES	YES
142	a	389.24	4.87348	YES	YES
143	a	389.47	4.68610	YES	YES
144	a	390.84	7.28676	YES	YES
145	a	390.94	6.67440	YES	YES
146	a	392.39	19.20476	YES	YES
147	a	393.35	8.40283	YES	YES
148	a	398.12	44.25761	YES	YES
149	a	407.77	4.98751	YES	YES
150	a	420.75	3.93021	YES	YES
151	a	428.83	2.94028	YES	YES
152	a	429.85	4.48234	YES	YES
153	a	430.56	13.40240	YES	YES
154	a	431.01	6.83862	YES	YES
155	a	431.93	8.25355	YES	YES
156	a	432.95	14.24129	YES	YES
157	a	433.81	4.75050	YES	YES

158	a	434.57	13.26186	YES	YES
159	a	436.39	13.70128	YES	YES
160	a	437.01	19.27017	YES	YES
161	a	459.55	23.79970	YES	YES
162	a	495.42	1.63065	YES	YES
163	a	529.91	6.57118	YES	YES
164	a	531.23	15.32237	YES	YES
165	a	557.33	17.15386	YES	YES
166	a	589.00	0.01103	YES	YES
167	a	589.71	0.45323	YES	YES
168	a	590.13	0.87949	YES	YES
169	a	590.67	0.03784	YES	YES
170	a	590.74	0.02176	YES	YES
171	a	591.03	0.07152	YES	YES
172	a	591.16	0.01956	YES	YES
173	a	598.21	4.02329	YES	YES
174	a	620.80	2.28516	YES	YES
175	a	623.42	20.02285	YES	YES
176	a	631.92	23.40019	YES	YES
177	a	632.08	14.85277	YES	YES
178	a	635.47	5.75188	YES	YES
179	a	636.13	10.37375	YES	YES
180	a	636.36	7.10544	YES	YES
181	a	636.74	13.79032	YES	YES
182	a	636.80	28.06712	YES	YES
183	a	637.34	1.06617	YES	YES
184	a	637.70	29.56243	YES	YES
185	a	647.72	6.81236	YES	YES
186	a	654.09	3.74039	YES	YES
187	a	663.35	0.47538	YES	YES
188	a	672.73	11.33157	YES	YES
189	a	673.22	11.69463	YES	YES
190	a	722.63	0.76123	YES	YES
191	a	737.89	5.32031	YES	YES
192	a	780.19	11.42311	YES	YES
193	a	804.75	8.46209	YES	YES
194	a	809.20	8.54832	YES	YES
195	a	813.58	14.11250	YES	YES
196	a	830.49	38.96877	YES	YES
197	a	834.79	0.04699	YES	YES
198	a	834.99	0.05570	YES	YES
199	a	835.23	0.02255	YES	YES
200	a	835.58	0.00437	YES	YES
201	a	837.20	0.09550	YES	YES
202	a	837.24	0.08660	YES	YES
203	a	837.86	0.51765	YES	YES
204	a	838.84	0.44337	YES	YES
205	a	840.79	0.24125	YES	YES
206	a	871.09	243.75947	YES	YES
207	a	923.14	36.58015	YES	YES
208	a	941.19	71.32564	YES	YES
209	a	949.15	228.90775	YES	YES
210	a	954.91	30.23325	YES	YES
211	a	956.83	33.81068	YES	YES
212	a	959.56	94.58564	YES	YES
213	a	962.30	471.65180	YES	YES
214	a	962.82	335.29531	YES	YES
215	a	963.96	421.29475	YES	YES
216	a	967.82	196.62366	YES	YES
217	a	978.89	517.66081	YES	YES
218	a	980.83	477.07846	YES	YES
219	a	981.09	129.72557	YES	YES
220	a	983.35	41.10821	YES	YES
221	a	984.66	62.84936	YES	YES
222	a	987.23	5.11531	YES	YES
223	a	987.78	21.27566	YES	YES
224	a	988.55	4.20936	YES	YES
225	a	989.23	7.06399	YES	YES
226	a	991.23	0.83522	YES	YES
227	a	1003.58	30.16225	YES	YES

228	a	1012.04	15.30264	YES	YES
229	a	1039.13	3.40841	YES	YES
230	a	1040.87	8.63165	YES	YES
231	a	1044.85	1.26261	YES	YES
232	a	1045.47	2.91062	YES	YES
233	a	1045.62	13.53931	YES	YES
234	a	1048.17	4.48991	YES	YES
235	a	1049.97	1.54060	YES	YES
236	a	1051.40	8.38013	YES	YES
237	a	1054.70	1.68244	YES	YES
238	a	1055.30	0.02793	YES	YES
239	a	1055.53	1.67519	YES	YES
240	a	1056.86	0.93881	YES	YES
241	a	1058.35	0.04039	YES	YES
242	a	1059.82	0.37218	YES	YES
243	a	1059.96	0.66688	YES	YES
244	a	1064.24	0.01745	YES	YES
245	a	1066.62	6.19149	YES	YES
246	a	1094.36	18.86372	YES	YES
247	a	1103.12	91.21436	YES	YES
248	a	1108.63	48.55552	YES	YES
249	a	1111.24	64.09569	YES	YES
250	a	1115.34	42.00615	YES	YES
251	a	1122.59	5.37040	YES	YES
252	a	1122.90	4.94010	YES	YES
253	a	1125.53	0.83680	YES	YES
254	a	1127.27	1.70538	YES	YES
255	a	1128.77	1.12880	YES	YES
256	a	1130.18	2.35422	YES	YES
257	a	1130.84	3.66006	YES	YES
258	a	1133.78	0.28319	YES	YES
259	a	1135.38	0.81233	YES	YES
260	a	1144.19	11.77348	YES	YES
261	a	1175.04	36.41126	YES	YES
262	a	1188.71	40.90904	YES	YES
263	a	1196.39	6.20904	YES	YES
264	a	1200.25	1.01617	YES	YES
265	a	1201.85	3.27148	YES	YES
266	a	1204.64	5.44904	YES	YES
267	a	1204.90	1.28333	YES	YES
268	a	1206.03	12.16053	YES	YES
269	a	1207.80	6.37831	YES	YES
270	a	1209.11	10.04483	YES	YES
271	a	1209.42	18.94280	YES	YES
272	a	1210.11	15.62600	YES	YES
273	a	1210.56	2.84117	YES	YES
274	a	1210.76	6.64158	YES	YES
275	a	1211.56	41.92684	YES	YES
276	a	1212.36	26.97546	YES	YES
277	a	1212.74	7.16191	YES	YES
278	a	1214.11	2.18081	YES	YES
279	a	1214.91	9.12912	YES	YES
280	a	1216.13	32.02929	YES	YES
281	a	1230.25	148.09806	YES	YES
282	a	1231.90	56.31084	YES	YES
283	a	1237.97	49.23102	YES	YES
284	a	1240.02	63.60391	YES	YES
285	a	1242.56	89.18875	YES	YES
286	a	1245.55	78.73078	YES	YES
287	a	1247.58	86.53828	YES	YES
288	a	1249.15	194.88393	YES	YES
289	a	1254.52	306.79475	YES	YES
290	a	1256.55	339.77028	YES	YES
291	a	1258.74	1005.02139	YES	YES
292	a	1260.93	333.36460	YES	YES
293	a	1261.04	115.95255	YES	YES
294	a	1261.52	557.93635	YES	YES
295	a	1262.73	94.66950	YES	YES
296	a	1262.79	255.69136	YES	YES
297	a	1263.64	98.18220	YES	YES

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   298        a            1264.00        67.00513       YES     YES
   299        a            1264.27        47.79465       YES     YES
   300        a            1264.86       137.15855       YES     YES
   301        a            1266.59        63.28869       YES     YES
   302        a            1267.72       228.01732       YES     YES
   303        a            1269.78       326.70913       YES     YES
   304        a            1281.03       100.82573       YES     YES
   305        a            1282.85       507.90070       YES     YES
   306        a            1285.38       181.81499       YES     YES
   307        a            1291.10        48.27757       YES     YES
   308        a            1300.77       116.07496       YES     YES
   309        a            1341.60       336.16956       YES     YES
   310        a            1347.47        53.12255       YES     YES
   311        a            1358.75       446.24738       YES     YES
   312        a            1377.60       138.40281       YES     YES
$end
```

$Al(OC_{10}F_{15})_3 \cdot OC_{10}F_{14}$ (2, zwitterionic)

```
Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:
C         -4.51497       -2.62121        2.74227
C         -4.56934       -1.32824        1.86224
C         -3.45714       -3.62307        2.16753
F         -5.73069       -3.21345        2.76483
F         -4.20027       -2.30891        4.01646
C         -4.95810       -1.70061        0.39851
C         -3.84245       -4.00273        0.70438
C         -3.87891       -2.68048       -0.18931
F         -5.02510       -0.59214       -0.35909
F         -6.16694       -2.29548        0.35309
F         -5.03250       -4.61766        0.65523
F         -2.92619       -4.83764        0.16520
C         -3.17445       -0.62121        1.85818
F         -5.50245       -0.47642        2.36754
C         -2.04729       -2.96072        2.16252
F         -3.43063       -4.74875        2.93224
C         -2.49187       -2.10559       -0.05851
F         -4.17399       -3.02539       -1.46188
C         -2.02667       -1.55243        1.23265
F         -2.83101       -0.29923        3.11366
F         -3.22949        0.51397        1.13860
F         -1.12209       -3.78605        1.64998
F         -1.66683       -2.60965        3.38831
F         -1.65282       -2.45904       -0.95938
O         -0.82733       -1.02487        1.34367
F          3.35144        1.52506        2.19729
F          3.09286        2.05792        4.72161
F          1.31933        0.54774        3.53596
F          4.12923        4.03892        3.05989
C          2.59418        2.60694        1.90169
F          3.02333        3.07075        0.70627
O          0.91140        1.26941        0.83391
C          2.35259        3.13941        4.38437
C          2.80915        3.69925        2.99946
C          0.63075        1.67033        3.21689
C          1.07547        2.19317        1.80289
F          2.55635        4.06372        5.35324
F          0.43968        2.26590        5.53015
C          0.84054        2.75368        4.31984
F         -0.68038        1.31483        3.18507
C          1.96426        4.96366        2.64904
F          2.36851        5.47837        1.46491
C          0.24224        3.49077        1.49061
F          0.59659        3.99104        0.28486
F          2.15972        5.93075        3.57753
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C         -0.00186        4.02111        3.96897
C          0.45008        4.58208        2.58477
F         -1.07696        3.17384        1.41119
F          0.15194        4.96318        4.92945
F         -1.32064        3.71235        3.94216
F         -0.28635        5.68989        2.27949
F          0.62622        0.02043       -3.16277
F          0.79422        2.19101       -4.56023
F          0.34690        2.32646       -1.99101
F         -0.36851       -0.04365       -5.74258
C         -0.70810       -0.00147       -3.37091
F         -1.08145       -1.30642       -3.37204
O         -1.22353        0.19835       -0.98929
C         -0.54155        2.12951       -4.75831
C         -1.02036        0.64056       -4.76043
C         -0.98427        2.26540       -2.24894
C         -1.44743        0.76394       -2.20680
F         -0.78234        2.69533       -5.96490
F         -0.87597        4.21615       -3.63502
C         -1.28844        2.91766       -3.63479
F         -1.60717        2.96354       -1.27493
C         -2.55781        0.58601       -5.02295
F         -2.98128       -0.70093       -5.04822
C         -2.98340        0.73631       -2.51345
F         -3.42302       -0.55798       -2.49104
F         -2.84843        1.11349       -6.23452
C         -2.82817        2.86134       -3.89888
C         -3.30581        1.37200       -3.90033
F         -3.66516        1.38677       -1.54642
F         -3.12006        3.44350       -5.08544
F         -3.49342        3.55936       -2.95025
F         -4.65050        1.32362       -4.12462
F          3.22123       -0.43382       -2.46030
F          4.64557       -2.42066       -3.33308
F          2.11450       -2.77915       -2.80978
F          5.86357       -0.58002       -1.63714
C          3.51865       -0.80156       -1.19174
F          3.52080        0.33421       -0.45350
O          1.18532       -1.24100       -0.68580
C          4.92611       -2.74163       -2.04875
C          4.93467       -1.45685       -1.15893
C          2.45078       -3.08240       -1.53460
C          2.42106       -1.78868       -0.64306
F          6.15472       -3.31281       -2.05343
F          3.86197       -4.87193       -2.28377
C          3.86387       -3.75125       -1.50553
F          1.51819       -3.96622       -1.09259
C          5.29079       -1.84433        0.31178
F          5.31636       -0.73916        1.09101
C          2.82378       -2.20619        0.81759
F          2.79042       -1.11523        1.62426
F          6.53010       -2.38797        0.36690
C          4.22991       -4.13937       -0.03723
C          4.23620       -2.85980        0.85984
F          1.90243       -3.06912        1.32105
F          5.44281       -4.74065        0.00083
F          3.33926       -5.04022        0.44262
F          4.55702       -3.20267        2.14084
Al         0.14481       -0.09892        0.12117

SCF energy GEOOPT =  -7952.999962689 H
ZPE =   1144. kJ/mol
FREEH energy =  1376.82 kJ/mol
FREEH entropy =   1.81847 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
```

3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.10	0.13167	YES	YES
8	a	13.89	0.03165	YES	YES
9	a	18.26	0.00968	YES	YES
10	a	20.45	0.29271	YES	YES
11	a	23.32	0.00474	YES	YES
12	a	24.27	0.10886	YES	YES
13	a	27.98	0.19230	YES	YES
14	a	31.71	0.41743	YES	YES
15	a	32.95	0.01932	YES	YES
16	a	36.52	0.19880	YES	YES
17	a	44.09	0.12385	YES	YES
18	a	47.15	2.41558	YES	YES
19	a	56.44	0.90912	YES	YES
20	a	61.58	1.80958	YES	YES
21	a	67.21	0.38170	YES	YES
22	a	69.50	0.17360	YES	YES
23	a	71.89	1.06341	YES	YES
24	a	87.13	0.59578	YES	YES
25	a	107.31	0.25624	YES	YES
26	a	129.91	0.31122	YES	YES
27	a	132.98	0.10352	YES	YES
28	a	135.01	0.08401	YES	YES
29	a	136.19	0.03293	YES	YES
30	a	137.02	0.00748	YES	YES
31	a	138.25	0.36714	YES	YES
32	a	140.42	0.59055	YES	YES
33	a	141.77	0.16113	YES	YES
34	a	142.26	0.06333	YES	YES
35	a	144.60	0.37434	YES	YES
36	a	157.64	1.09041	YES	YES
37	a	163.22	0.73346	YES	YES
38	a	182.30	0.83159	YES	YES
39	a	187.17	1.49857	YES	YES
40	a	192.04	0.68727	YES	YES
41	a	194.30	0.80298	YES	YES
42	a	195.30	0.71271	YES	YES
43	a	196.16	0.18526	YES	YES
44	a	196.83	0.08455	YES	YES
45	a	197.91	0.02118	YES	YES
46	a	199.30	0.35351	YES	YES
47	a	201.23	0.34786	YES	YES
48	a	202.35	0.08251	YES	YES
49	a	202.67	0.03469	YES	YES
50	a	203.88	0.23402	YES	YES
51	a	205.12	0.04867	YES	YES
52	a	205.42	0.03715	YES	YES
53	a	206.45	0.12725	YES	YES
54	a	208.44	0.05619	YES	YES
55	a	209.36	0.24070	YES	YES
56	a	214.55	0.10518	YES	YES
57	a	225.01	0.00086	YES	YES
58	a	225.18	0.00644	YES	YES
59	a	227.09	0.00110	YES	YES
60	a	228.26	0.11381	YES	YES
61	a	234.15	1.37469	YES	YES
62	a	240.38	0.15342	YES	YES
63	a	242.90	0.06644	YES	YES
64	a	243.66	0.34780	YES	YES
65	a	244.36	0.51658	YES	YES
66	a	244.68	0.59373	YES	YES
67	a	244.76	0.39956	YES	YES
68	a	244.90	0.25853	YES	YES
69	a	245.80	0.10588	YES	YES
70	a	246.09	0.04139	YES	YES
71	a	246.29	0.58445	YES	YES
72	a	246.53	0.19109	YES	YES

73	a	246.75	0.06169	YES	YES
74	a	247.32	0.08785	YES	YES
75	a	247.50	0.03976	YES	YES
76	a	247.76	0.50164	YES	YES
77	a	248.36	0.16113	YES	YES
78	a	248.52	0.15785	YES	YES
79	a	249.03	0.19624	YES	YES
80	a	250.49	2.68636	YES	YES
81	a	251.93	1.86749	YES	YES
82	a	252.64	3.01299	YES	YES
83	a	252.83	0.10051	YES	YES
84	a	253.72	1.96794	YES	YES
85	a	255.71	0.70581	YES	YES
86	a	256.34	0.59986	YES	YES
87	a	257.88	0.26358	YES	YES
88	a	258.15	0.55622	YES	YES
89	a	258.88	0.14749	YES	YES
90	a	259.08	0.32681	YES	YES
91	a	262.45	1.50243	YES	YES
92	a	262.90	0.22382	YES	YES
93	a	263.28	0.08132	YES	YES
94	a	263.49	0.04191	YES	YES
95	a	263.68	0.18317	YES	YES
96	a	267.03	2.77430	YES	YES
97	a	271.19	1.13339	YES	YES
98	a	275.05	1.87382	YES	YES
99	a	277.59	4.98383	YES	YES
100	a	281.43	3.99630	YES	YES
101	a	284.62	23.38211	YES	YES
102	a	290.29	3.77983	YES	YES
103	a	291.63	1.18857	YES	YES
104	a	294.09	2.35787	YES	YES
105	a	295.38	3.39517	YES	YES
106	a	296.72	6.26431	YES	YES
107	a	296.88	5.77427	YES	YES
108	a	297.28	2.23939	YES	YES
109	a	297.74	0.18703	YES	YES
110	a	298.18	1.05526	YES	YES
111	a	298.22	7.00807	YES	YES
112	a	299.03	4.08096	YES	YES
113	a	299.71	17.09823	YES	YES
114	a	300.68	2.42523	YES	YES
115	a	303.01	7.73767	YES	YES
116	a	303.64	0.61577	YES	YES
117	a	306.87	0.93039	YES	YES
118	a	310.92	0.30628	YES	YES
119	a	314.92	2.91082	YES	YES
120	a	317.99	3.92469	YES	YES
121	a	321.57	20.32920	YES	YES
122	a	335.35	16.40395	YES	YES
123	a	338.99	12.73207	YES	YES
124	a	362.40	0.48204	YES	YES
125	a	363.30	1.11363	YES	YES
126	a	364.43	1.12324	YES	YES
127	a	365.64	7.19116	YES	YES
128	a	367.23	0.02401	YES	YES
129	a	370.24	5.18836	YES	YES
130	a	372.46	3.48849	YES	YES
131	a	376.90	1.01030	YES	YES
132	a	377.25	2.52515	YES	YES
133	a	377.89	0.08250	YES	YES
134	a	378.21	0.28802	YES	YES
135	a	378.54	0.65496	YES	YES
136	a	379.12	0.36972	YES	YES
137	a	379.40	0.07509	YES	YES
138	a	379.96	0.58654	YES	YES
139	a	380.75	2.07354	YES	YES
140	a	381.97	0.44705	YES	YES
141	a	382.93	2.83797	YES	YES
142	a	386.01	0.57354	YES	YES

143	a	387.80	0.71170	YES	YES
144	a	388.92	2.37412	YES	YES
145	a	389.35	9.31928	YES	YES
146	a	390.48	7.90610	YES	YES
147	a	394.79	17.49414	YES	YES
148	a	401.22	30.03890	YES	YES
149	a	404.47	9.08925	YES	YES
150	a	416.01	14.92684	YES	YES
151	a	425.16	0.42961	YES	YES
152	a	429.84	3.73965	YES	YES
153	a	430.83	9.17864	YES	YES
154	a	431.28	19.36684	YES	YES
155	a	432.51	4.31853	YES	YES
156	a	432.88	1.61266	YES	YES
157	a	433.20	12.74090	YES	YES
158	a	434.45	16.03234	YES	YES
159	a	435.53	25.23911	YES	YES
160	a	439.74	11.52021	YES	YES
161	a	464.35	6.33629	YES	YES
162	a	494.37	6.50038	YES	YES
163	a	518.09	25.65345	YES	YES
164	a	526.65	7.93058	YES	YES
165	a	529.34	9.08099	YES	YES
166	a	534.75	6.84322	YES	YES
167	a	576.12	18.14595	YES	YES
168	a	587.59	0.09766	YES	YES
169	a	588.72	0.04481	YES	YES
170	a	589.03	0.03438	YES	YES
171	a	590.38	0.09624	YES	YES
172	a	590.78	0.02321	YES	YES
173	a	590.93	0.11686	YES	YES
174	a	610.44	5.01855	YES	YES
175	a	616.88	26.58967	YES	YES
176	a	627.71	4.73668	YES	YES
177	a	630.72	26.05011	YES	YES
178	a	631.11	16.74066	YES	YES
179	a	634.90	4.14092	YES	YES
180	a	635.26	4.22898	YES	YES
181	a	635.58	18.47132	YES	YES
182	a	635.87	7.44525	YES	YES
183	a	636.70	9.70330	YES	YES
184	a	637.13	9.01589	YES	YES
185	a	647.25	2.49364	YES	YES
186	a	650.86	8.04768	YES	YES
187	a	658.61	20.64560	YES	YES
188	a	667.86	12.15348	YES	YES
189	a	671.36	7.13216	YES	YES
190	a	686.86	143.62569	YES	YES
191	a	699.81	47.29844	YES	YES
192	a	720.10	31.44306	YES	YES
193	a	756.37	10.52023	YES	YES
194	a	790.57	0.82003	YES	YES
195	a	799.02	10.93857	YES	YES
196	a	822.18	1.83523	YES	YES
197	a	832.92	2.22027	YES	YES
198	a	834.55	0.11624	YES	YES
199	a	834.76	0.00981	YES	YES
200	a	834.88	0.45270	YES	YES
201	a	835.64	0.01478	YES	YES
202	a	836.22	0.01118	YES	YES
203	a	836.24	0.00640	YES	YES
204	a	837.70	0.04216	YES	YES
205	a	839.69	0.11345	YES	YES
206	a	842.18	0.08704	YES	YES
207	a	911.07	19.09811	YES	YES
208	a	948.75	18.29098	YES	YES
209	a	954.60	54.81114	YES	YES
210	a	956.88	52.77461	YES	YES
211	a	958.38	102.89000	YES	YES
212	a	960.26	232.28097	YES	YES

213	a	962.21	307.71023	YES	YES
214	a	963.92	454.21481	YES	YES
215	a	967.13	608.35005	YES	YES
216	a	973.92	478.14230	YES	YES
217	a	978.21	408.53510	YES	YES
218	a	979.25	180.02026	YES	YES
219	a	981.91	265.46304	YES	YES
220	a	985.07	5.91982	YES	YES
221	a	985.84	12.22650	YES	YES
222	a	986.05	16.33658	YES	YES
223	a	987.73	13.62572	YES	YES
224	a	989.34	10.91330	YES	YES
225	a	989.50	4.92775	YES	YES
226	a	1007.12	83.05885	YES	YES
227	a	1015.62	89.24731	YES	YES
228	a	1024.41	40.24485	YES	YES
229	a	1036.93	7.46930	YES	YES
230	a	1038.30	7.08947	YES	YES
231	a	1039.00	10.99128	YES	YES
232	a	1041.63	2.93267	YES	YES
233	a	1043.42	4.71162	YES	YES
234	a	1047.37	5.84637	YES	YES
235	a	1051.62	10.67779	YES	YES
236	a	1054.81	1.12172	YES	YES
237	a	1055.11	0.84558	YES	YES
238	a	1056.30	0.07816	YES	YES
239	a	1056.64	0.59799	YES	YES
240	a	1056.75	0.75610	YES	YES
241	a	1057.84	0.30569	YES	YES
242	a	1058.11	0.32188	YES	YES
243	a	1059.19	2.51332	YES	YES
244	a	1062.34	0.73972	YES	YES
245	a	1062.71	0.46886	YES	YES
246	a	1090.22	42.30708	YES	YES
247	a	1101.81	69.75624	YES	YES
248	a	1110.10	87.16532	YES	YES
249	a	1118.18	5.57168	YES	YES
250	a	1121.58	1.93905	YES	YES
251	a	1124.46	2.39855	YES	YES
252	a	1126.26	10.52944	YES	YES
253	a	1126.81	1.24901	YES	YES
254	a	1128.58	5.66914	YES	YES
255	a	1128.81	53.94567	YES	YES
256	a	1130.59	13.50238	YES	YES
257	a	1132.87	1.51690	YES	YES
258	a	1133.14	1.52164	YES	YES
259	a	1137.70	13.11499	YES	YES
260	a	1147.24	20.08656	YES	YES
261	a	1189.95	65.09662	YES	YES
262	a	1192.75	44.72960	YES	YES
263	a	1197.78	11.22951	YES	YES
264	a	1199.54	23.53702	YES	YES
265	a	1199.90	18.15152	YES	YES
266	a	1202.59	5.24845	YES	YES
267	a	1204.09	15.05964	YES	YES
268	a	1205.06	19.23687	YES	YES
269	a	1206.01	1.75264	YES	YES
270	a	1206.87	15.70605	YES	YES
271	a	1208.32	32.56135	YES	YES
272	a	1208.78	7.03179	YES	YES
273	a	1209.42	4.15418	YES	YES
274	a	1210.82	3.58156	YES	YES
275	a	1211.15	1.42008	YES	YES
276	a	1211.57	10.29869	YES	YES
277	a	1212.61	1.12774	YES	YES
278	a	1212.82	6.30209	YES	YES
279	a	1214.57	1.60539	YES	YES
280	a	1219.33	39.72679	YES	YES
281	a	1229.93	68.83291	YES	YES
282	a	1236.15	45.28273	YES	YES

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   283        a            1236.56        35.23834       YES     YES
   284        a            1238.00        24.54282       YES     YES
   285        a            1244.48       130.71768       YES     YES
   286        a            1247.06        76.75789       YES     YES
   287        a            1251.54       549.99195       YES     YES
   288        a            1254.06       269.88388       YES     YES
   289        a            1256.60      1188.76474       YES     YES
   290        a            1258.79       409.07878       YES     YES
   291        a            1259.63        52.46526       YES     YES
   292        a            1260.12        87.19133       YES     YES
   293        a            1260.43       223.01346       YES     YES
   294        a            1261.06       178.95557       YES     YES
   295        a            1261.49        69.70305       YES     YES
   296        a            1261.70       136.88102       YES     YES
   297        a            1262.40       177.80461       YES     YES
   298        a            1263.20       200.78514       YES     YES
   299        a            1263.96        20.20113       YES     YES
   300        a            1264.25        45.66873       YES     YES
   301        a            1269.00       229.66245       YES     YES
   302        a            1274.96       248.87235       YES     YES
   303        a            1276.62       277.27757       YES     YES
   304        a            1279.46       244.01062       YES     YES
   305        a            1282.75       186.35272       YES     YES
   306        a            1289.09        99.17900       YES     YES
   307        a            1305.76        75.08728       YES     YES
   308        a            1313.28        20.24380       YES     YES
   309        a            1348.43       207.54688       YES     YES
   310        a            1369.24       250.69726       YES     YES
   311        a            1397.88        17.91668       YES     YES
   312        a            1446.15       124.94641       YES     YES
$end
```

$[Al(OC(CF_3)_3)_4]^-$

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Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: s4

Cartesian coordinates in Ångström:
Al    0.0000000   -0.0000000    0.0000000
F    -3.0318554    0.2835492   -2.8010363
F    -1.3017983   -0.5233695   -3.8393431
F    -3.1714460   -1.6490024   -3.7991377
F    -3.4518196   -3.3803642   -1.6507739
F    -4.1876720   -1.4211006   -1.0380896
F    -2.8155783   -2.5093424    0.2473285
F     0.3980426   -2.0380367   -2.2716481
F    -1.1078741   -3.3315586   -3.1781520
F    -0.6538372   -3.4993708   -1.0540349
O    -1.3936644   -0.5604766   -0.9199578
C    -0.7956366   -2.6220052   -2.0673923
C    -2.3603431   -0.8461888   -3.0669893
C    -3.1028286   -2.2243431   -1.0299070
C    -1.8775625   -1.5254099   -1.7295068
F     0.2835492    3.0318554    2.8010363
F     3.0318554   -0.2835492   -2.8010363
F    -0.2835492   -3.0318554    2.8010363
F    -0.5233695    1.3017983    3.8393431
F     1.3017983    0.5233695   -3.8393431
F     0.5233695   -1.3017983    3.8393431
F    -1.6490024    3.1714460    3.7991377
F     3.1714460    1.6490024   -3.7991377
F     1.6490024   -3.1714460    3.7991377
F    -3.3803642    3.4518196    1.6507739
F     3.4518196    3.3803642   -1.6507739
F     3.3803642   -3.4518196    1.6507739
F    -1.4211006    4.1876720    1.0380896
F     4.1876720    1.4211006   -1.0380896
F     1.4211006   -4.1876720    1.0380896
```

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F    -2.5093424    2.8155783   -0.2473285
F     2.8155783    2.5093424    0.2473285
F     2.5093424   -2.8155783   -0.2473285
F    -2.0380367   -0.3980426    2.2716481
F    -0.3980426    2.0380367   -2.2716481
F     2.0380367    0.3980426    2.2716481
F    -3.3315586    1.1078741    3.1781520
F     1.1078741    3.3315586   -3.1781520
F     3.3315586   -1.1078741    3.1781520
F    -3.4993708    0.6538372    1.0540349
F     0.6538372    3.4993708   -1.0540349
F     3.4993708   -0.6538372    1.0540349
O    -0.5604766    1.3936644    0.9199578
O     1.3936644    0.5604766   -0.9199578
O     0.5604766   -1.3936644    0.9199578
C    -2.6220052    0.7956366    2.0673923
C     0.7956366    2.6220052   -2.0673923
C     2.6220052   -0.7956366    2.0673923
C    -0.8461888    2.3603431    3.0669893
C     2.3603431    0.8461888   -3.0669893
C     0.8461888   -2.3603431    3.0669893
C    -2.2243431    3.1028286    1.0299070
C     3.1028286    2.2243431   -1.0299070
C     2.2243431   -3.1028286    1.0299070
C    -1.5254099    1.8775625    1.7295068
C     1.8775625    1.5254099   -1.7295068
C     1.5254099   -1.8775625    1.7295068

SCF energy GEOOPT =  -4744.673250758 H
ZPE =   575.2 kJ/mol
FREEH energy =   721.13 kJ/mol
FREEH entropy =   1.33929 kJ/mol/K

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
     4                      -0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        e             14.90         0.00000       YES     YES
     8        e             14.90         0.00000       YES     YES
     9        b             17.22         0.02465       YES     YES
    10        b             21.33         0.00000       YES     YES
    11        b             24.14         0.11889       YES     YES
    12        e             31.43         0.00413       YES     YES
    13        e             31.43         0.00413       YES     YES
    14        a             32.03         0.00000       NO      YES
    15        b             43.59         0.06350       YES     YES
    16        e             44.89         0.05709       YES     YES
    17        e             44.89         0.05709       YES     YES
    18        a             59.09         0.00000       NO      YES
    19        a             61.20         0.00000       NO      YES
    20        b             71.06         0.72890       YES     YES
    21        b             73.81         0.00354       YES     YES
    22        e             74.00         0.04166       YES     YES
    23        e             74.00         0.04166       YES     YES
    24        b             77.27         0.00239       YES     YES
    25        e             77.69         0.18302       YES     YES
    26        e             77.69         0.18302       YES     YES
    27        a             79.31         0.00000       NO      YES
    28        a             80.05         0.00000       NO      YES
    29        e             82.79         0.45566       YES     YES
    30        e             82.79         0.45566       YES     YES
    31        b             88.15         0.01083       YES     YES
    32        a             90.60         0.00000       NO      YES
    33        e             94.75         0.62857       YES     YES
    34        e             94.75         0.62857       YES     YES
```

35	b	97.65	1.32279	YES	YES
36	a	110.95	0.00000	NO	YES
37	e	153.19	0.48109	YES	YES
38	e	153.19	0.48109	YES	YES
39	a	157.72	0.00000	NO	YES
40	b	159.55	0.06053	YES	YES
41	e	162.22	1.02701	YES	YES
42	e	162.22	1.02701	YES	YES
43	a	163.96	0.00000	NO	YES
44	b	164.43	1.10831	YES	YES
45	b	189.58	5.55404	YES	YES
46	e	193.24	2.97926	YES	YES
47	e	193.24	2.97926	YES	YES
48	a	215.82	0.00000	NO	YES
49	e	262.42	1.14305	YES	YES
50	e	262.42	1.14305	YES	YES
51	b	271.13	3.44089	YES	YES
52	a	272.23	0.00000	NO	YES
53	e	277.89	3.97711	YES	YES
54	e	277.89	3.97711	YES	YES
55	b	283.51	2.52914	YES	YES
56	a	283.56	0.00000	NO	YES
57	e	284.71	0.03784	YES	YES
58	e	284.71	0.03784	YES	YES
59	b	285.11	0.12510	YES	YES
60	b	285.70	0.00000	YES	YES
61	b	304.12	12.25182	YES	YES
62	e	304.33	8.59729	YES	YES
63	e	304.33	8.59729	YES	YES
64	a	310.72	0.00000	NO	YES
65	e	314.55	0.01921	YES	YES
66	e	314.55	0.01921	YES	YES
67	a	318.70	0.00000	NO	YES
68	b	319.54	1.16277	YES	YES
69	e	322.85	1.04054	YES	YES
70	e	322.85	1.04054	YES	YES
71	b	324.71	1.93166	YES	YES
72	a	326.38	0.00000	NO	YES
73	e	343.29	1.61838	YES	YES
74	e	343.29	1.61838	YES	YES
75	b	349.45	4.62833	YES	YES
76	e	355.14	10.58430	YES	YES
77	e	355.14	10.58430	YES	YES
78	a	355.89	0.00000	NO	YES
79	b	372.13	50.65808	YES	YES
80	a	390.92	0.00000	NO	YES
81	b	434.16	39.26935	YES	YES
82	e	450.06	62.07331	YES	YES
83	e	450.06	62.07330	YES	YES
84	a	516.40	0.00000	NO	YES
85	a	518.51	0.00000	NO	YES
86	e	518.93	3.97843	YES	YES
87	e	518.93	3.97843	YES	YES
88	b	519.47	8.21447	YES	YES
89	a	520.90	0.00000	NO	YES
90	e	520.91	11.74333	YES	YES
91	e	520.91	11.74333	YES	YES
92	b	522.07	6.59957	YES	YES
93	b	524.24	0.19663	YES	YES
94	e	524.31	0.88448	YES	YES
95	e	524.31	0.88448	YES	YES
96	a	527.56	0.00000	NO	YES
97	b	544.67	18.23423	YES	YES
98	e	551.79	13.26018	YES	YES
99	e	551.79	13.26018	YES	YES
100	e	554.27	0.21168	YES	YES
101	e	554.27	0.21168	YES	YES
102	b	554.52	0.46673	YES	YES
103	a	554.79	0.00000	NO	YES
104	b	556.93	0.00000	YES	YES

105	b	557.24	1.61506	YES	YES
106	e	561.71	23.49230	YES	YES
107	e	561.71	23.49229	YES	YES
108	e	707.56	0.92153	YES	YES
109	e	707.56	0.92153	YES	YES
110	a	707.91	0.00000	NO	YES
111	a	709.00	0.00000	NO	YES
112	b	709.16	43.93581	YES	YES
113	e	710.23	88.94851	YES	YES
114	e	710.23	88.94852	YES	YES
115	b	710.27	40.84483	YES	YES
116	a	725.27	0.00000	NO	YES
117	b	736.62	1.28589	YES	YES
118	e	738.39	4.85046	YES	YES
119	e	738.39	4.85046	YES	YES
120	a	778.11	0.00000	NO	YES
121	b	813.95	13.58564	YES	YES
122	e	830.17	26.65696	YES	YES
123	e	830.17	26.65696	YES	YES
124	e	957.58	3.52236	YES	YES
125	e	957.58	3.52236	YES	YES
126	a	958.12	0.00000	NO	YES
127	b	961.60	70.04680	YES	YES
128	a	962.77	0.00000	NO	YES
129	e	965.50	364.26241	YES	YES
130	e	965.50	364.26239	YES	YES
131	b	966.06	239.25263	YES	YES
132	b	1110.83	18.96430	YES	YES
133	e	1113.22	5.97870	YES	YES
134	e	1113.22	5.97871	YES	YES
135	a	1121.13	0.00000	NO	YES
136	e	1132.61	12.53091	YES	YES
137	e	1132.61	12.53091	YES	YES
138	a	1135.20	0.00000	NO	YES
139	a	1139.16	0.00000	NO	YES
140	b	1139.43	30.51715	YES	YES
141	b	1141.70	0.90289	YES	YES
142	e	1143.76	12.52315	YES	YES
143	e	1143.76	12.52315	YES	YES
144	a	1193.78	0.00000	NO	YES
145	e	1198.48	18.67923	YES	YES
146	e	1198.48	18.67923	YES	YES
147	b	1200.61	2.02006	YES	YES
148	a	1203.03	0.00000	NO	YES
149	e	1210.29	3.87515	YES	YES
150	e	1210.29	3.87515	YES	YES
151	b	1214.51	1.58844	YES	YES
152	b	1218.17	938.24895	YES	YES
153	e	1219.37	756.90704	YES	YES
154	e	1219.37	756.90677	YES	YES
155	e	1230.30	612.79532	YES	YES
156	e	1230.30	612.79568	YES	YES
157	b	1234.03	655.08511	YES	YES
158	a	1241.20	0.00000	NO	YES
159	e	1242.07	251.71110	YES	YES
160	e	1242.07	251.71081	YES	YES
161	a	1246.49	0.00000	NO	YES
162	b	1253.94	0.00000	YES	YES
163	b	1253.96	222.50119	YES	YES
164	a	1260.67	0.00000	NO	YES
165	e	1263.95	925.79401	YES	YES
166	e	1263.95	925.79422	YES	YES
167	b	1268.36	778.90369	YES	YES
168	b	1339.15	301.57597	YES	YES
169	e	1340.76	235.84951	YES	YES
170	e	1340.76	235.84948	YES	YES
171	a	1362.87	0.00000	NO	YES

$end

$[Al(OC(CF_3)_3)_3 \cdot OCF_2C(CF_3)_2$

Method: (RI-)BP86(D3BJ)/def-SV(P)
Symmetry: c1

Cartesian coordinates in Ångström:

Al	0.23919	-0.09613	0.12304
O	-1.20560	0.85608	-0.97519
F	-3.60797	2.27389	-0.35043
F	-1.45058	-1.41230	-2.42397
F	-3.39807	-1.68276	-1.48263
F	-0.87892	1.16663	-3.25463
C	-3.72008	0.99263	-0.72079
F	-3.25677	-0.69100	-3.41955
F	-4.82527	0.85677	-1.48178
F	-1.71115	2.80917	-2.10733
C	-2.51094	0.53605	-1.56478
C	-2.65065	-0.86152	-2.22822
C	-1.56521	1.50379	-2.18018
O	1.19260	-0.76266	-1.14402
C	2.33213	-0.73126	-1.88890
C	3.47775	-1.49841	-1.13235
F	3.24454	-2.82408	-1.13919
F	4.68385	-1.27789	-1.68841
C	2.78753	0.75070	-2.16595
F	1.70858	1.51238	-2.45098
F	3.37817	1.28203	-1.07966
F	3.64397	0.83593	-3.19828
C	2.01493	-1.45476	-3.24990
F	3.13343	-1.76080	-3.93365
F	1.24919	-0.66105	-4.02980
F	1.33152	-2.58539	-3.02286
F	1.04433	3.65320	-0.41878
F	-1.34105	-3.60380	-0.36818
O	0.86509	1.33704	0.82688
C	1.43267	3.64406	0.86950
F	2.77132	3.53545	0.89669
F	1.09122	4.82440	1.42504
C	0.75922	2.43630	1.61989
C	1.50892	2.15911	2.97522
F	1.75990	3.29390	3.65435
F	0.75975	1.35399	3.75857
F	2.67107	1.53472	2.73904
O	-1.06405	-1.15135	0.65382
C	-1.72169	-3.44616	0.90835
F	-3.05635	-3.28728	0.93168
F	-1.41713	-4.57029	1.59073
C	-1.00256	-2.20022	1.53634
C	-1.70829	-1.78075	2.87812
F	-1.93469	-2.83854	3.68005
F	-0.92683	-0.90237	3.54278
F	-2.87658	-1.18122	2.62040
C	-0.75014	2.77596	1.90742
F	-1.43905	1.63118	2.11520
F	-1.31329	3.38706	0.84308
F	-0.90874	3.56745	2.97816
C	0.50191	-2.56625	1.82639
F	1.22097	-1.37049	1.73153
F	1.02006	-3.38151	0.90622
F	0.73020	-3.06914	3.03469
F	3.52407	-1.09948	0.15297
F	-3.83642	0.23899	0.37425

SCF energy GEOOPT = -4644.688081095 H
ZPE = 568.5 kJ/mol
FREEH energy = 711.58 kJ/mol
FREEH entropy = 1.32480 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.46	0.01906	YES	YES
8	a	17.27	0.04686	YES	YES
9	a	21.34	0.02363	YES	YES
10	a	23.21	0.00743	YES	YES
11	a	26.30	0.12129	YES	YES
12	a	31.58	0.08239	YES	YES
13	a	36.91	0.38358	YES	YES
14	a	38.01	0.16547	YES	YES
15	a	41.99	0.07654	YES	YES
16	a	43.26	0.34544	YES	YES
17	a	49.85	0.07459	YES	YES
18	a	54.87	0.40412	YES	YES
19	a	58.62	0.42102	YES	YES
20	a	62.30	0.76571	YES	YES
21	a	64.37	0.42459	YES	YES
22	a	69.16	0.11501	YES	YES
23	a	69.63	0.11706	YES	YES
24	a	71.74	0.30463	YES	YES
25	a	74.80	0.12648	YES	YES
26	a	77.01	0.10003	YES	YES
27	a	77.99	0.48555	YES	YES
28	a	81.37	1.42618	YES	YES
29	a	84.65	0.66127	YES	YES
30	a	87.82	0.26554	YES	YES
31	a	88.59	0.30928	YES	YES
32	a	95.76	7.64030	YES	YES
33	a	97.32	1.62730	YES	YES
34	a	105.13	3.16466	YES	YES
35	a	114.23	0.51720	YES	YES
36	a	139.28	0.85269	YES	YES
37	a	153.59	2.23192	YES	YES
38	a	156.17	4.08061	YES	YES
39	a	159.20	0.39656	YES	YES
40	a	161.91	0.46485	YES	YES
41	a	163.19	0.51025	YES	YES
42	a	164.21	2.03299	YES	YES
43	a	167.14	1.25177	YES	YES
44	a	171.36	1.58814	YES	YES
45	a	175.67	4.70662	YES	YES
46	a	187.69	6.39115	YES	YES
47	a	190.37	8.57127	YES	YES
48	a	209.26	22.88400	YES	YES
49	a	240.77	57.95425	YES	YES
50	a	270.28	0.76538	YES	YES
51	a	272.36	2.27037	YES	YES
52	a	275.19	8.46972	YES	YES
53	a	280.20	23.64346	YES	YES
54	a	281.79	11.12953	YES	YES
55	a	284.77	5.49127	YES	YES
56	a	285.34	0.15654	YES	YES
57	a	285.87	1.68501	YES	YES
58	a	286.88	0.45027	YES	YES
59	a	297.43	6.17281	YES	YES
60	a	297.82	0.43011	YES	YES
61	a	306.87	6.45398	YES	YES
62	a	308.77	6.05333	YES	YES
63	a	312.08	0.25823	YES	YES
64	a	314.77	0.30339	YES	YES
65	a	317.38	0.48210	YES	YES
66	a	318.58	0.88600	YES	YES
67	a	320.85	2.75547	YES	YES
68	a	321.62	0.87764	YES	YES

69	a	323.37	0.95766	YES	YES
70	a	325.98	0.80762	YES	YES
71	a	327.94	5.27449	YES	YES
72	a	338.36	0.80109	YES	YES
73	a	352.59	0.50090	YES	YES
74	a	354.68	5.09241	YES	YES
75	a	357.59	10.13906	YES	YES
76	a	365.72	22.69918	YES	YES
77	a	369.73	6.27271	YES	YES
78	a	412.81	27.62121	YES	YES
79	a	444.06	43.73060	YES	YES
80	a	459.95	1.89539	YES	YES
81	a	475.72	8.84408	YES	YES
82	a	508.45	5.07362	YES	YES
83	a	511.11	1.17160	YES	YES
84	a	511.78	7.89118	YES	YES
85	a	518.88	4.70583	YES	YES
86	a	519.93	4.78414	YES	YES
87	a	520.50	2.74594	YES	YES
88	a	520.85	2.62854	YES	YES
89	a	521.81	6.70254	YES	YES
90	a	522.95	5.57271	YES	YES
91	a	525.23	1.86867	YES	YES
92	a	525.74	0.76430	YES	YES
93	a	528.11	2.65887	YES	YES
94	a	529.02	1.34672	YES	YES
95	a	552.73	0.67544	YES	YES
96	a	553.86	2.96975	YES	YES
97	a	554.25	2.22198	YES	YES
98	a	555.22	1.24889	YES	YES
99	a	555.66	0.45413	YES	YES
100	a	556.63	2.52048	YES	YES
101	a	557.69	0.43568	YES	YES
102	a	562.88	6.59105	YES	YES
103	a	564.82	12.35858	YES	YES
104	a	590.64	8.37944	YES	YES
105	a	592.61	25.90913	YES	YES
106	a	700.31	20.63844	YES	YES
107	a	704.97	26.79309	YES	YES
108	a	708.92	33.89863	YES	YES
109	a	709.39	2.25017	YES	YES
110	a	709.41	34.45002	YES	YES
111	a	710.97	28.05666	YES	YES
112	a	711.59	60.61332	YES	YES
113	a	714.84	80.36223	YES	YES
114	a	724.59	1.65247	YES	YES
115	a	740.54	0.93815	YES	YES
116	a	742.30	0.52799	YES	YES
117	a	760.69	0.12960	YES	YES
118	a	786.88	7.88998	YES	YES
119	a	798.18	6.74486	YES	YES
120	a	868.52	19.86607	YES	YES
121	a	891.46	12.06566	YES	YES
122	a	938.22	159.56622	YES	YES
123	a	962.16	36.51571	YES	YES
124	a	963.52	58.33078	YES	YES
125	a	967.61	166.30377	YES	YES
126	a	970.29	174.55185	YES	YES
127	a	971.89	103.55045	YES	YES
128	a	978.73	190.93007	YES	YES
129	a	993.52	231.45336	YES	YES
130	a	1042.88	300.54355	YES	YES
131	a	1063.97	39.21732	YES	YES
132	a	1109.30	3.13385	YES	YES
133	a	1115.76	0.87458	YES	YES
134	a	1145.11	30.03806	YES	YES
135	a	1156.21	12.44857	YES	YES
136	a	1158.80	11.25783	YES	YES
137	a	1162.82	24.05041	YES	YES
138	a	1163.93	1.02499	YES	YES

```
   139        a             1169.36        20.40706       YES      YES
   140        a             1172.11        10.71589       YES      YES
   141        a             1174.62        28.01324       YES      YES
   142        a             1183.10       193.67927       YES      YES
   143        a             1191.95         4.73924       YES      YES
   144        a             1194.19        40.31285       YES      YES
   145        a             1201.51        11.25186       YES      YES
   146        a             1203.34       152.27618       YES      YES
   147        a             1206.30        14.73368       YES      YES
   148        a             1211.97       421.50416       YES      YES
   149        a             1213.53        98.02469       YES      YES
   150        a             1219.54        61.59254       YES      YES
   151        a             1227.26       532.97439       YES      YES
   152        a             1228.23       213.56140       YES      YES
   153        a             1241.24       121.76507       YES      YES
   154        a             1244.83       261.97058       YES      YES
   155        a             1247.88       358.44184       YES      YES
   156        a             1251.71       567.62203       YES      YES
   157        a             1254.88      1071.34269       YES      YES
   158        a             1260.86       588.10343       YES      YES
   159        a             1262.91       424.74259       YES      YES
   160        a             1266.18       579.13754       YES      YES
   161        a             1269.94       296.93044       YES      YES
   162        a             1278.50       203.77527       YES      YES
   163        a             1287.55       499.58510       YES      YES
   164        a             1308.55         1.23406       YES      YES
   165        a             1334.71       294.52446       YES      YES
   166        a             1345.60       296.23454       YES      YES
   167        a             1355.86       183.01741       YES      YES
   168        a             1464.26       396.98952       YES      YES
$end
```

One-electron reduction of the [*pfAd*]$^-$ anion

Note that the calculated values for $[Al(OC(CF_3)_3)_4]^-$, $[Al(OCH(CF_3)_2)_4]^-$ and $[B(OCH(CF_3)_2)_4]^-$ are taken from reference [34].

The gas phase calculations were first performed at RI-B3LYP(D3BJ)/def2-TZVPP level of theory (grid m5, 298.15 K). Afterwards, COSMO values were obtained by running a single point calculation at RI-B3LYP(D3BJ)/def2-TZVPP level of theory (grid m5, 298.15 K) with 1,2-dimethoxyethane with $\varepsilon_r = 7.30$[33].

Table S- 13: Calculated thermodynamic data at RI-B3LYP(D3BJ)/def2-TZVPP level of theory (grid m5, 298.15 K) for the [*pfAd*]$^-$ anion and [*pfAd*]$^{2-}$ dianion in the gas phase and in solution (COSMO, 1,2-dimethoxyethane with $\varepsilon_r = 7.30$[33]):

	E_{SCF} / H	E_{SCF} / kJ·mol^{-1}	E_{vrt} / kJ·mol^{-1}	$S°$ / kJ·mol^{-1}	$G°$ / kJ·mol^{-1}	$H°$ / kJ·mol^{-1}
$[Al(OC_{10}F_{15})_4]^-$	-8058.73	-21158187.53	1405.76	1.80967	-21157318.85	-21156779.29
$[Al(OC_{10}F_{15})_4]^{\cdot 2-}$	-8058.67	-21158034.80	1374.44	1.83685	-21157205.54	-21156657.89
$[Al(OC_{10}F_{15})_4]^-$ COSMO	-8058.76	-21158275.22	1405.76	1.80967	-21157406.53	-21156866.98
$[Al(OC_{10}F_{15})_4]^{\cdot 2-}$ COSMO	-8058.80	-21158366.60	1374.44	1.83685	-21157537.34	-21156989.68

Detailed results for the calculation of the one-electron reduction of the [*pfAd*]$^-$ anion

$[Al(OC_{10}F_{15})_4]^-$

```
Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: c1
```

Cartesian coordinates in Ångström:

C	-1.1185127	-1.4882533	5.5877734
C	-2.1739519	-0.8345338	4.6514499
C	-0.3021809	-2.5448015	4.7904636
F	-1.7251734	-2.0659681	6.6484427
F	-0.2996624	-0.5510501	6.1011496
C	-3.1369997	-1.9302027	4.1117525
C	-1.2664063	-3.6412202	4.2540955
C	-2.3229233	-2.9895324	3.3161980
F	-4.0826520	-1.3807649	3.3284531
F	-3.7988924	-2.5173590	5.1336055
F	-1.8775842	-4.2721895	5.2812738
F	-0.5769484	-4.5930254	3.5983764
C	-1.4508065	-0.1443055	3.4564027
F	-2.8905237	0.0830972	5.3571507
C	0.4196160	-1.8526279	3.5938896
F	0.6135165	-3.1202530	5.6178759
C	-1.5969778	-2.3011969	2.1228229
F	-3.1684069	-3.9524348	2.8572169
C	-0.6098732	-1.1769519	2.6128708
F	-0.6539883	0.8349139	3.9282353
F	-2.3647536	0.4609386	2.6753481
F	1.1627745	-2.7644753	2.9372590
F	1.2852694	-0.9356346	4.0692507
F	-2.5107702	-1.7767042	1.2812716
F	-0.9298698	-3.2326637	1.4159131
O	0.0422236	-0.5867173	1.6094085
F	4.0672632	0.9283227	-0.6971251
F	5.5593723	1.6452992	1.3021933
F	3.2471320	0.5158469	1.7751643
F	5.5542255	3.2336556	-0.9691589
C	3.4542738	2.1266007	-0.6505912
F	3.0957270	2.4175871	-1.9167289
O	1.3281160	1.1466437	-0.1987255
C	4.9306859	2.8355973	1.2932133
C	4.4692497	3.1969474	-0.1472244
C	2.6777911	1.7365371	1.7336743
C	2.1810093	2.0551302	0.2740222
F	5.8389223	3.7341838	1.7342805
F	4.1069757	2.4958096	3.4990949
C	3.6971351	2.8030156	2.2380152
F	1.6349454	1.6999212	2.5835518
C	3.7892276	4.5953181	-0.1363144
F	3.4215129	4.9486449	-1.3822146
C	1.5410743	3.4932765	0.3011829
F	1.1170283	3.8367778	-0.9303470
F	4.6657771	5.5408653	0.2691022
C	3.0167639	4.2026443	2.2483199
C	2.5535974	4.5637533	0.8083862
F	0.4491918	3.4976041	1.0924952
F	3.8754753	5.1371141	2.7137124
F	1.9703402	4.2140087	3.0938100
F	1.9684152	5.7929832	0.8208820
F	-1.8557706	-0.0108425	-2.9691978
F	-2.6093787	1.8862508	-4.5573341
F	-1.0322148	2.4393183	-2.5453398
F	-4.4071941	-0.1476422	-3.9963913
C	-2.9080718	0.2436497	-2.1699856
F	-3.2559029	-0.9322382	-1.6111057
O	-1.5228977	0.8462543	-0.2669014
C	-3.6570463	2.0969218	-3.7399568
C	-4.0851401	0.7716236	-3.0456312
C	-2.1256726	2.6235492	-1.7776266
C	-2.5077665	1.2791756	-1.0532619
F	-4.6536412	2.5544724	-4.5301978
F	-2.9321466	4.3149790	-3.2709146
C	-3.2959559	3.1546403	-2.6587106
F	-1.7964224	3.5631437	-0.8705041
C	-5.3269447	1.0361825	-2.1493528

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F    -5.7400708   -0.1075214   -1.5719350
C    -3.7951040    1.5607901   -0.1904316
F    -4.1926478    0.4376951    0.4376281
F    -6.3664463    1.4658305   -2.8987971
C    -4.5394975    3.4178972   -1.7615096
C    -4.9678697    2.0940476   -1.0674073
F    -3.5209925    2.4584066    0.7768014
F    -5.5567303    3.9102431   -2.5027669
F    -4.2666018    4.3630363   -0.8424769
F    -6.0613735    2.3296903   -0.2909427
F     0.6501092   -0.8643932   -3.9075407
F     0.6500116   -3.0978150   -5.2429110
F    -0.9160454   -2.8471627   -3.1764387
F     3.0444848   -1.7340616   -4.9685062
C     1.5966759   -1.3739678   -3.0944776
F     2.3492739   -0.3312310   -2.6970743
O     0.1396798   -1.2360025   -1.1730960
C     1.6083584   -3.5475904   -4.4111785
C     2.4838549   -2.3678898   -3.9019728
C     0.0858094   -3.2861706   -2.3894288
C     0.9301035   -2.0722613   -1.8484245
F     2.3548264   -4.4055535   -5.1415934
F     0.2148602   -5.3199627   -3.6491530
C     0.9724888   -4.2826944   -3.1971983
F    -0.4997329   -3.9415085   -1.3683180
C     3.6119111   -2.9187416   -2.9837421
F     4.4054240   -1.9179213   -2.5613458
C     2.0888155   -2.6657934   -0.9633501
F     2.8532066   -1.6675294   -0.4761030
F     4.4130368   -3.7578164   -3.6774008
C     2.1020095   -4.8355659   -2.2819273
C     2.9787769   -3.6566507   -1.7702825
F     1.5792308   -3.3023684    0.1079244
F     2.8617481   -5.7250929   -2.9589864
F     1.5766328   -5.5166059   -1.2467907
F     3.9703802   -4.1473712   -0.9774484
Al   -0.0032010    0.0499964   -0.0096065

SCF energy GEOOPT =  -8058.728455869 H
ZPE =   1176. kJ/mol
FREEH energy =  1405.76 kJ/mol
FREEH entropy =   1.80967 kJ/mol/K
COSMO energy + OC. Corr. =  -8058.7618544614 H

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000         -       -
     2                      -0.00         0.00000         -       -
     3                      -0.00         0.00000         -       -
     4                      -0.00         0.00000         -       -
     5                       0.00         0.00000         -       -
     6                       0.00         0.00000         -       -
     7        a              9.20         0.00301       YES     YES
     8        a             12.33         0.00281       YES     YES
     9        a             15.31         0.03398       YES     YES
    10        a             18.10         0.00388       YES     YES
    11        a             19.71         0.00113       YES     YES
    12        a             20.59         0.03607       YES     YES
    13        a             23.14         0.05888       YES     YES
    14        a             23.39         0.04605       YES     YES
    15        a             24.64         0.03398       YES     YES
    16        a             28.27         0.00882       YES     YES
    17        a             39.17         0.02873       YES     YES
    18        a             43.79         0.00014       YES     YES
    19        a             56.74         0.02484       YES     YES
    20        a             57.32         0.03096       YES     YES
    21        a             68.27         0.52176       YES     YES
    22        a             68.93         0.58955       YES     YES
    23        a             69.73         0.57266       YES     YES
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24	a	89.82	0.00028	YES	YES
25	a	137.46	0.01833	YES	YES
26	a	138.24	0.00678	YES	YES
27	a	138.83	0.01804	YES	YES
28	a	139.57	0.02260	YES	YES
29	a	141.03	0.00411	YES	YES
30	a	141.11	0.00792	YES	YES
31	a	143.20	0.00604	YES	YES
32	a	144.33	0.02201	YES	YES
33	a	145.22	0.33592	YES	YES
34	a	146.47	0.30035	YES	YES
35	a	147.89	0.02379	YES	YES
36	a	148.24	0.45592	YES	YES
37	a	200.33	0.33965	YES	YES
38	a	200.74	0.46852	YES	YES
39	a	201.15	0.42824	YES	YES
40	a	201.31	0.11875	YES	YES
41	a	202.09	0.25596	YES	YES
42	a	202.49	0.04175	YES	YES
43	a	203.31	0.00254	YES	YES
44	a	204.48	0.18395	YES	YES
45	a	204.94	0.13860	YES	YES
46	a	205.20	0.02300	YES	YES
47	a	206.35	0.30869	YES	YES
48	a	208.37	0.06572	YES	YES
49	a	211.23	0.03288	YES	YES
50	a	211.62	0.07402	YES	YES
51	a	212.13	0.04333	YES	YES
52	a	212.28	0.08122	YES	YES
53	a	212.60	0.09559	YES	YES
54	a	213.58	0.00015	YES	YES
55	a	213.67	0.05571	YES	YES
56	a	214.61	0.04932	YES	YES
57	a	231.35	0.00168	YES	YES
58	a	231.38	0.00120	YES	YES
59	a	231.54	0.00122	YES	YES
60	a	231.77	0.00499	YES	YES
61	a	250.49	0.01080	YES	YES
62	a	250.75	0.02500	YES	YES
63	a	250.78	0.04077	YES	YES
64	a	251.38	0.01901	YES	YES
65	a	251.44	0.01261	YES	YES
66	a	251.57	0.00518	YES	YES
67	a	251.71	0.00665	YES	YES
68	a	251.84	0.00204	YES	YES
69	a	251.96	0.00361	YES	YES
70	a	252.13	0.06325	YES	YES
71	a	252.42	0.01854	YES	YES
72	a	252.74	0.00497	YES	YES
73	a	253.49	0.06167	YES	YES
74	a	254.54	0.44591	YES	YES
75	a	255.13	0.85909	YES	YES
76	a	255.67	1.20222	YES	YES
77	a	256.03	0.22949	YES	YES
78	a	256.11	0.49855	YES	YES
79	a	256.15	0.27409	YES	YES
80	a	256.39	0.11532	YES	YES
81	a	263.44	4.19622	YES	YES
82	a	263.75	5.05565	YES	YES
83	a	263.88	4.09507	YES	YES
84	a	264.70	0.38335	YES	YES
85	a	266.63	0.66136	YES	YES
86	a	267.62	0.86750	YES	YES
87	a	269.72	0.06229	YES	YES
88	a	270.53	0.59899	YES	YES
89	a	271.55	0.23618	YES	YES
90	a	271.86	0.12758	YES	YES
91	a	271.99	0.00132	YES	YES
92	a	272.47	0.46410	YES	YES
93	a	277.19	0.00986	YES	YES

94	a	277.30	0.01479	YES	YES
95	a	277.42	0.13040	YES	YES
96	a	277.50	0.03352	YES	YES
97	a	281.64	0.39133	YES	YES
98	a	282.46	0.89966	YES	YES
99	a	285.12	5.18299	YES	YES
100	a	289.92	13.23960	YES	YES
101	a	291.25	16.68418	YES	YES
102	a	299.54	0.33236	YES	YES
103	a	300.55	0.94945	YES	YES
104	a	303.71	15.71440	YES	YES
105	a	304.05	3.86218	YES	YES
106	a	304.19	3.61315	YES	YES
107	a	304.36	6.84610	YES	YES
108	a	304.75	6.07660	YES	YES
109	a	305.20	2.94008	YES	YES
110	a	305.55	3.87365	YES	YES
111	a	305.61	2.18618	YES	YES
112	a	305.78	0.01563	YES	YES
113	a	305.88	2.76264	YES	YES
114	a	305.93	2.22809	YES	YES
115	a	306.50	18.02570	YES	YES
116	a	308.77	0.32797	YES	YES
117	a	311.03	0.29465	YES	YES
118	a	311.67	1.25684	YES	YES
119	a	314.81	0.18139	YES	YES
120	a	319.65	2.48423	YES	YES
121	a	320.93	3.17053	YES	YES
122	a	325.61	0.20315	YES	YES
123	a	331.51	0.60679	YES	YES
124	a	350.19	18.80093	YES	YES
125	a	366.67	2.06481	YES	YES
126	a	367.05	0.68806	YES	YES
127	a	368.13	1.16274	YES	YES
128	a	369.17	0.57655	YES	YES
129	a	382.53	33.30288	YES	YES
130	a	385.51	1.89174	YES	YES
131	a	385.57	10.69480	YES	YES
132	a	385.90	3.02673	YES	YES
133	a	386.05	2.97781	YES	YES
134	a	386.15	1.31211	YES	YES
135	a	386.71	0.39984	YES	YES
136	a	387.10	0.02326	YES	YES
137	a	387.21	1.37760	YES	YES
138	a	387.43	0.11015	YES	YES
139	a	387.63	2.03916	YES	YES
140	a	388.27	0.03821	YES	YES
141	a	388.35	0.74705	YES	YES
142	a	389.22	9.50462	YES	YES
143	a	391.94	7.17451	YES	YES
144	a	397.72	0.48884	YES	YES
145	a	398.09	0.51834	YES	YES
146	a	398.26	0.12613	YES	YES
147	a	399.13	0.00962	YES	YES
148	a	400.51	19.74288	YES	YES
149	a	401.10	8.06181	YES	YES
150	a	402.73	33.36992	YES	YES
151	a	406.59	43.55010	YES	YES
152	a	438.44	0.09087	YES	YES
153	a	439.97	8.67172	YES	YES
154	a	440.06	9.20459	YES	YES
155	a	440.15	14.72035	YES	YES
156	a	442.22	2.88716	YES	YES
157	a	442.67	2.61701	YES	YES
158	a	443.46	0.64057	YES	YES
159	a	443.82	13.68480	YES	YES
160	a	444.46	22.23780	YES	YES
161	a	444.72	41.99354	YES	YES
162	a	445.22	9.07007	YES	YES
163	a	447.12	48.76170	YES	YES

164	a	502.55	0.01048	YES	YES
165	a	532.30	10.77384	YES	YES
166	a	533.16	15.18527	YES	YES
167	a	535.38	19.16718	YES	YES
168	a	604.28	0.09064	YES	YES
169	a	604.80	0.05552	YES	YES
170	a	605.21	0.08785	YES	YES
171	a	605.26	0.01813	YES	YES
172	a	606.03	0.03239	YES	YES
173	a	606.07	0.00560	YES	YES
174	a	606.39	0.08699	YES	YES
175	a	606.46	0.00007	YES	YES
176	a	626.82	0.10012	YES	YES
177	a	640.86	18.06125	YES	YES
178	a	641.52	8.62024	YES	YES
179	a	642.40	16.53937	YES	YES
180	a	649.12	2.75975	YES	YES
181	a	649.33	0.02495	YES	YES
182	a	649.58	19.31563	YES	YES
183	a	649.65	12.60420	YES	YES
184	a	650.21	5.05859	YES	YES
185	a	650.38	16.57797	YES	YES
186	a	650.71	24.02149	YES	YES
187	a	650.88	10.01310	YES	YES
188	a	665.07	0.01367	YES	YES
189	a	679.04	18.17859	YES	YES
190	a	679.51	18.04943	YES	YES
191	a	680.10	18.08519	YES	YES
192	a	726.25	0.00707	YES	YES
193	a	762.90	14.88315	YES	YES
194	a	764.07	21.46995	YES	YES
195	a	768.65	18.78694	YES	YES
196	a	852.11	0.07814	YES	YES
197	a	852.17	0.00604	YES	YES
198	a	852.25	0.01402	YES	YES
199	a	852.42	0.22480	YES	YES
200	a	854.30	0.12041	YES	YES
201	a	854.34	0.05239	YES	YES
202	a	854.44	0.06557	YES	YES
203	a	854.59	0.04652	YES	YES
204	a	854.70	0.45977	YES	YES
205	a	854.75	0.07289	YES	YES
206	a	854.84	0.05133	YES	YES
207	a	855.11	0.01652	YES	YES
208	a	963.39	10.94226	YES	YES
209	a	963.67	9.07540	YES	YES
210	a	965.19	1.46380	YES	YES
211	a	969.01	5.75001	YES	YES
212	a	970.73	40.46971	YES	YES
213	a	971.91	779.62729	YES	YES
214	a	972.79	709.15942	YES	YES
215	a	972.98	750.16324	YES	YES
216	a	984.44	596.38964	YES	YES
217	a	984.57	484.30739	YES	YES
218	a	985.17	589.99409	YES	YES
219	a	991.45	0.47159	YES	YES
220	a	992.49	11.98566	YES	YES
221	a	992.89	16.49877	YES	YES
222	a	993.34	10.47331	YES	YES
223	a	994.18	29.07953	YES	YES
224	a	994.38	2.11064	YES	YES
225	a	994.65	27.74602	YES	YES
226	a	995.28	6.46651	YES	YES
227	a	995.95	16.23423	YES	YES
228	a	1038.89	0.57613	YES	YES
229	a	1040.08	0.55837	YES	YES
230	a	1040.19	3.33708	YES	YES
231	a	1040.88	0.61444	YES	YES
232	a	1041.36	0.75243	YES	YES
233	a	1041.66	2.70915	YES	YES

234	a	1042.34	1.53996	YES	YES
235	a	1042.52	0.46587	YES	YES
236	a	1069.01	0.11852	YES	YES
237	a	1069.07	0.14363	YES	YES
238	a	1069.56	0.06550	YES	YES
239	a	1069.74	0.09886	YES	YES
240	a	1069.98	0.16312	YES	YES
241	a	1070.17	0.13802	YES	YES
242	a	1070.27	0.04775	YES	YES
243	a	1070.42	0.18567	YES	YES
244	a	1082.66	0.07795	YES	YES
245	a	1083.27	0.91290	YES	YES
246	a	1083.61	0.99350	YES	YES
247	a	1083.85	0.32115	YES	YES
248	a	1104.46	80.08523	YES	YES
249	a	1105.28	71.78489	YES	YES
250	a	1107.43	84.39655	YES	YES
251	a	1112.02	3.41281	YES	YES
252	a	1133.61	0.20613	YES	YES
253	a	1134.51	0.70550	YES	YES
254	a	1134.86	0.17504	YES	YES
255	a	1134.97	0.16805	YES	YES
256	a	1135.74	0.24576	YES	YES
257	a	1135.81	2.01191	YES	YES
258	a	1136.37	0.34618	YES	YES
259	a	1136.59	1.00857	YES	YES
260	a	1145.97	0.22803	YES	YES
261	a	1146.93	0.11707	YES	YES
262	a	1147.34	0.11439	YES	YES
263	a	1147.80	0.09966	YES	YES
264	a	1215.26	2.16112	YES	YES
265	a	1216.49	1.39661	YES	YES
266	a	1216.61	3.31079	YES	YES
267	a	1217.28	1.44254	YES	YES
268	a	1218.75	6.54080	YES	YES
269	a	1222.00	1.80562	YES	YES
270	a	1223.03	3.25682	YES	YES
271	a	1223.21	8.25315	YES	YES
272	a	1225.43	0.29431	YES	YES
273	a	1225.74	1.14163	YES	YES
274	a	1226.05	0.36262	YES	YES
275	a	1227.44	0.71172	YES	YES
276	a	1228.18	2.03657	YES	YES
277	a	1228.79	1.64051	YES	YES
278	a	1229.27	0.56950	YES	YES
279	a	1233.14	0.81880	YES	YES
280	a	1233.82	22.13006	YES	YES
281	a	1234.08	1.32430	YES	YES
282	a	1235.14	24.96467	YES	YES
283	a	1235.29	28.34508	YES	YES
284	a	1260.87	76.44086	YES	YES
285	a	1261.06	80.38828	YES	YES
286	a	1261.18	62.57638	YES	YES
287	a	1262.80	0.04923	YES	YES
288	a	1266.70	15.76235	YES	YES
289	a	1267.66	5.24042	YES	YES
290	a	1269.39	694.87200	YES	YES
291	a	1269.70	1051.10622	YES	YES
292	a	1270.19	991.48437	YES	YES
293	a	1270.79	311.36917	YES	YES
294	a	1273.79	39.10336	YES	YES
295	a	1274.63	29.70113	YES	YES
296	a	1275.01	30.14021	YES	YES
297	a	1276.00	385.30553	YES	YES
298	a	1276.16	265.31689	YES	YES
299	a	1276.42	286.67155	YES	YES
300	a	1277.88	4.53117	YES	YES
301	a	1278.57	32.16670	YES	YES
302	a	1279.11	25.27405	YES	YES
303	a	1279.55	12.61022	YES	YES

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   304        a            1281.63       198.77545       YES     YES
   305        a            1282.73       218.49718       YES     YES
   306        a            1282.84       107.11342       YES     YES
   307        a            1283.53       101.66968       YES     YES
   308        a            1296.95       131.92098       YES     YES
   309        a            1297.09       125.81423       YES     YES
   310        a            1297.28       143.12073       YES     YES
   311        a            1304.78         0.13314       YES     YES
   312        a            1363.13       413.00871       YES     YES
   313        a            1366.91       393.17947       YES     YES
   314        a            1370.90       479.76705       YES     YES
   315        a            1405.04         7.20023       YES     YES
$end
```

$[Al(OC_{10}F_{15})_4]^{\cdot 2-}$

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Method: (RI-)B3LYP(D3BJ)/def2-TZVPP
Symmetry: c1

Cartesian coordinates in Ångström:
C    -1.1184943   -1.4949780    5.5965137
C    -2.1742651   -0.8512523    4.6645446
C    -0.3059900   -2.5448050    4.7992041
F    -1.7203238   -2.0740997    6.6692412
F    -0.2997633   -0.5518757    6.1118065
C    -3.1331931   -1.9456744    4.1330594
C    -1.2618283   -3.6434477    4.2712981
C    -2.3183335   -2.9974724    3.3403153
F    -4.0895820   -1.4011956    3.3530583
F    -3.7960197   -2.5363310    5.1631452
F    -1.8684536   -4.2826527    5.3067151
F    -0.5694842   -4.5996855    3.6159435
C    -1.4616646   -0.1558549    3.4687717
F    -2.9031253    0.0836884    5.3816842
C     0.4127517   -1.8546348    3.6034387
F     0.6343886   -3.1245184    5.6378698
C    -1.6034598   -2.3121689    2.1406686
F    -3.1750038   -3.9805464    2.8741988
C    -0.6175334   -1.1820957    2.6204273
F    -0.6665526    0.8300950    3.9387220
F    -2.3825239    0.4470205    2.6904890
F     1.1605932   -2.7666464    2.9463408
F     1.2797713   -0.9333119    4.0767692
F    -2.5252314   -1.7940902    1.3004103
F    -0.9348394   -3.2449944    1.4317131
O     0.0316290   -0.5892991    1.6126459
F     4.0727215    0.9374393   -0.6887655
F     5.5668664    1.6568335    1.3085944
F     3.2554482    0.5308273    1.7850438
F     5.5742033    3.2393506   -0.9775317
C     3.4592159    2.1383973   -0.6412987
F     3.1013994    2.4283037   -1.9114695
O     1.3274867    1.1550578   -0.1911866
C     4.9333212    2.8497110    1.2966127
C     4.4705631    3.2077420   -0.1371327
C     2.6845393    1.7537749    1.7405995
C     2.1837066    2.0656700    0.2806866
F     5.8513816    3.7504170    1.7380229
F     4.1194069    2.5075259    3.5200293
C     3.7038656    2.8214956    2.2362532
F     1.6415992    1.7178291    2.5938375
C     3.7977201    4.6021457   -0.1307268
F     3.4313121    4.9586062   -1.3814584
C     1.5511605    3.5073914    0.3073609
F     1.1254760    3.8514995   -0.9266219
F     4.6809804    5.5548712    0.2704939
C     3.0288166    4.2163597    2.2468496
C     2.5686323    4.5714460    0.8113719
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F     0.4573339    3.5179660    1.1000188
F     3.8916588    5.1571164    2.7154776
F     1.9814895    4.2343229    3.0978599
F     1.9712247    5.8225814    0.8206329
F    -1.8667891   -0.0014863   -2.9867635
F    -2.6201311    1.9033528   -4.5684590
F    -1.0429949    2.4503277   -2.5562259
F    -4.4209065   -0.1447631   -4.0252843
C    -2.9203713    0.2541370   -2.1858176
F    -3.2716710   -0.9258205   -1.6308013
O    -1.5291011    0.8448926   -0.2763345
C    -3.6689720    2.1107296   -3.7447373
C    -4.0955336    0.7900160   -3.0555777
C    -2.1385029    2.6295459   -1.7859609
C    -2.5155958    1.2823717   -1.0637149
F    -4.6685953    2.5740621   -4.5416732
F    -2.9358272    4.3420679   -3.2797566
C    -3.3104180    3.1585150   -2.6621897
F    -1.8082208    3.5690751   -0.8748356
C    -5.3336616    1.0490193   -2.1638735
F    -5.7533517   -0.0995879   -1.5901337
C    -3.8063717    1.5636598   -0.2054189
F    -4.2062345    0.4380917    0.4225158
F    -6.3814730    1.4810771   -2.9151303
C    -4.5485796    3.4208665   -1.7690974
C    -4.9732354    2.0989431   -1.0841349
F    -3.5335915    2.4603983    0.7677020
F    -5.5718647    3.9227997   -2.5105205
F    -4.2780989    4.3688981   -0.8450865
F    -6.0858593    2.3357019   -0.2892814
F     0.6644233   -0.8724723   -3.9171826
F     0.6529581   -3.1062596   -5.2516158
F    -0.9095349   -2.8488633   -3.1847378
F     3.0590866   -1.7437164   -4.9910160
C     1.6104427   -1.3877866   -3.1018375
F     2.3698246   -0.3464081   -2.7069960
O     0.1505414   -1.2367315   -1.1769423
C     1.6119459   -3.5590682   -4.4147000
C     2.4891193   -2.3889851   -3.9059099
C     0.0943071   -3.2911042   -2.3968231
C     0.9392133   -2.0779938   -1.8536008
F     2.3551687   -4.4248815   -5.1537831
F     0.1988091   -5.3377726   -3.6615210
C     0.9783478   -4.2866186   -3.2032747
F    -0.4958882   -3.9464680   -1.3746425
C     3.6132013   -2.9417105   -2.9943974
F     4.4177345   -1.9439870   -2.5740701
C     2.0982129   -2.6800023   -0.9741217
F     2.8710713   -1.6857236   -0.4863240
F     4.4167334   -3.7876810   -3.6928135
C     2.1003447   -4.8452611   -2.2931646
C     2.9778478   -3.6734387   -1.7861187
F     1.5871829   -3.3163980    0.0999678
F     2.8580862   -5.7468459   -2.9725536
F     1.5728708   -5.5299302   -1.2558142
F     3.9835984   -4.1754244   -0.9779892
Al   -0.0046951    0.0507873   -0.0099749

SCF energy GEOOPT =  -8058.670284998 H
ZPE =   1141. kJ/mol
FREEH energy =  1374.44 kJ/mol
FREEH entropy =   1.83685 kJ/mol/K
COSMO energy + OC. Corr. =  -8058.7966583963 H

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                      -0.00         0.00000        -       -
     2                      -0.00         0.00000        -       -
     3                      -0.00         0.00000        -       -
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4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	8.67	0.00254	YES	YES
8	a	11.63	0.00506	YES	YES
9	a	14.49	0.06347	YES	YES
10	a	17.41	0.04848	YES	YES
11	a	18.76	0.02102	YES	YES
12	a	19.65	0.20638	YES	YES
13	a	22.04	0.57968	YES	YES
14	a	22.34	0.43949	YES	YES
15	a	23.58	0.27803	YES	YES
16	a	26.80	2.12015	YES	YES
17	a	37.46	1.68328	YES	YES
18	a	42.21	0.10596	YES	YES
19	a	56.07	0.44946	YES	YES
20	a	56.54	0.85592	YES	YES
21	a	66.01	21.80096	YES	YES
22	a	66.40	24.04280	YES	YES
23	a	67.20	24.37028	YES	YES
24	a	88.24	0.02787	YES	YES
25	a	136.92	0.44133	YES	YES
26	a	137.62	0.09013	YES	YES
27	a	138.22	0.37523	YES	YES
28	a	138.95	0.36806	YES	YES
29	a	140.25	0.19096	YES	YES
30	a	140.37	0.28736	YES	YES
31	a	142.38	1.15711	YES	YES
32	a	143.59	0.75092	YES	YES
33	a	144.12	7.79101	YES	YES
34	a	145.31	7.08951	YES	YES
35	a	146.71	4.44560	YES	YES
36	a	146.90	8.57822	YES	YES
37	a	199.09	0.43606	YES	YES
38	a	199.40	0.38163	YES	YES
39	a	199.69	0.80196	YES	YES
40	a	199.99	0.57245	YES	YES
41	a	200.67	2.20784	YES	YES
42	a	200.95	4.54142	YES	YES
43	a	201.86	1.70887	YES	YES
44	a	202.54	7.41264	YES	YES
45	a	203.13	5.32807	YES	YES
46	a	203.48	0.33209	YES	YES
47	a	204.49	6.28931	YES	YES
48	a	206.18	1.33452	YES	YES
49	a	212.54	0.39841	YES	YES
50	a	213.19	6.23436	YES	YES
51	a	213.25	0.90138	YES	YES
52	a	213.44	2.58700	YES	YES
53	a	213.61	2.64553	YES	YES
54	a	214.54	3.11820	YES	YES
55	a	214.92	0.02371	YES	YES
56	a	215.49	2.17032	YES	YES
57	a	233.12	0.19074	YES	YES
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62	a	249.47	70.71468	YES	YES
63	a	249.51	239.81690	YES	YES
64	a	250.24	234.91423	YES	YES
65	a	250.41	130.16516	YES	YES
66	a	250.79	63.99511	YES	YES
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71	a	251.88	112.91374	YES	YES
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73	a	252.24	133.68094	YES	YES

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99	a	283.29	107.36995	YES	YES
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103	a	295.85	7.73220	YES	YES
104	a	297.04	23.89267	YES	YES
105	a	298.23	116.81178	YES	YES
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107	a	299.31	46.86155	YES	YES
108	a	303.01	3.04988	YES	YES
109	a	303.56	6.37031	YES	YES
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123	a	326.24	72.92050	YES	YES
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125	a	358.83	2176.05961	YES	YES
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135	a	383.53	10.86321	YES	YES
136	a	383.61	6.06163	YES	YES
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166	a	476.16	3652.86019	YES	YES
167	a	486.72	32.66023	YES	YES
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170	a	598.85	4.72404	YES	YES
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173	a	599.76	0.27196	YES	YES
174	a	600.04	0.64104	YES	YES
175	a	600.11	0.50776	YES	YES
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178	a	626.16	801.94597	YES	YES
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184	a	636.52	3.21147	YES	YES
185	a	636.70	1.69073	YES	YES
186	a	636.76	12.48741	YES	YES
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191	a	666.77	96.22706	YES	YES
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195	a	702.39	0.43610	YES	YES
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201	a	840.08	20.02477	YES	YES
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203	a	840.57	16.49313	YES	YES
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206	a	842.14	88.13240	YES	YES
207	a	842.43	60.24049	YES	YES
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212	a	918.76	97.80417	YES	YES
213	a	921.46	247.05313	YES	YES

214	a	923.03	87.52450	YES	YES
215	a	925.48	318.15825	YES	YES
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222	a	973.13	11.34988	YES	YES
223	a	973.60	80.63833	YES	YES
224	a	974.23	118.65535	YES	YES
225	a	975.78	26.18261	YES	YES
226	a	977.62	15.46758	YES	YES
227	a	979.24	185.80190	YES	YES
228	a	980.95	367.70653	YES	YES
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230	a	982.83	636.21626	YES	YES
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232	a	993.77	26.12347	YES	YES
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234	a	994.65	1.58859	YES	YES
235	a	995.06	32.72456	YES	YES
236	a	995.62	14.92751	YES	YES
237	a	996.33	50.02098	YES	YES
238	a	996.92	58.50921	YES	YES
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240	a	1051.32	2.55849	YES	YES
241	a	1051.86	3.03986	YES	YES
242	a	1052.35	2.99895	YES	YES
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244	a	1053.60	7.34755	YES	YES
245	a	1053.88	12.70900	YES	YES
246	a	1054.04	7.29612	YES	YES
247	a	1081.20	1.36444	YES	YES
248	a	1083.43	0.27218	YES	YES
249	a	1084.26	5.04330	YES	YES
250	a	1084.65	4.05775	YES	YES
251	a	1084.97	1.32425	YES	YES
252	a	1092.21	603.71867	YES	YES
253	a	1093.20	558.11262	YES	YES
254	a	1094.27	598.27116	YES	YES
255	a	1121.18	22.64043	YES	YES
256	a	1121.38	13.46062	YES	YES
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258	a	1121.98	4.29995	YES	YES
259	a	1123.12	6.95714	YES	YES
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261	a	1123.91	9.88528	YES	YES
262	a	1124.11	5.92973	YES	YES
263	a	1154.93	32.35582	YES	YES
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265	a	1155.57	16.35532	YES	YES
266	a	1156.26	59.10792	YES	YES
267	a	1156.58	34.28889	YES	YES
268	a	1156.92	52.88672	YES	YES
269	a	1157.64	213.67076	YES	YES
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271	a	1158.32	95.22973	YES	YES
272	a	1159.58	246.00794	YES	YES
273	a	1160.57	418.43576	YES	YES
274	a	1161.88	280.32420	YES	YES
275	a	1179.45	2.55427	YES	YES
276	a	1192.37	3.72419	YES	YES
277	a	1193.01	14.52057	YES	YES
278	a	1193.93	35.86410	YES	YES
279	a	1194.42	10.99293	YES	YES
280	a	1195.26	8.13801	YES	YES
281	a	1196.93	8.89357	YES	YES
282	a	1198.72	24.69568	YES	YES
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   291        a             1210.86         6.46087       YES     YES
   292        a             1212.16         1.22562       YES     YES
   293        a             1213.55         7.64900       YES     YES
   294        a             1214.30         8.48287       YES     YES
   295        a             1214.94        21.44426       YES     YES
   296        a             1233.10       736.59618       YES     YES
   297        a             1233.82       682.14162       YES     YES
   298        a             1234.53       785.58383       YES     YES
   299        a             1250.26       518.99165       YES     YES
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   302        a             1251.69        52.72198       YES     YES
   303        a             1257.16        39.20360       YES     YES
   304        a             1259.08         3.29158       YES     YES
   305        a             1262.52        11.52897       YES     YES
   306        a             1265.07       273.03281       YES     YES
   307        a             1271.17       624.10150       YES     YES
   308        a             1271.62       124.69334       YES     YES
   309        a             1271.78       687.23574       YES     YES
   310        a             1272.73       433.99576       YES     YES
   311        a             1281.31         3.47804       YES     YES
   312        a             1302.21        25.25530       YES     YES
   313        a             1305.61         1.82213       YES     YES
   314        a             1307.28        19.34043       YES     YES
   315        a             1374.62         0.04763       YES     YES
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