SUPPORTING INFORMATION

Fluoride ion chelation *via* pnictogen bonding using a distibora [1.1]ferrocenophane

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1. Synthetic details

1.1 General considerations:

Antimony is potentially toxic and should be handled with caution. 1,1′-dilithioferrocene·(tmeda)[1] and $PhSbCl_2$[2] were prepared using existing synthetic methods. 3,4,5,6-tetrachloro-1,2-benzoquinone (*o*-chloranil) was purchased from Acros Organics and tetra-*n*-butylammonium difluorotriphenylsilicate (TBAT) was purchased from TCI. Both were used as received. Unless otherwise noted, all preparations were carried out under an atmosphere of dry N_2 employing either a glovebox or standard Schlenk techniques. Solvents were dried by refluxing under N_2 over Na/K (Et_2O and THF) and CaH_2 (CH_2Cl_2). All other solvents were ACS reagent grade and used as received. NMR spectra were recorded on a Bruker Ascend 400 FT NMR (399.51 MHz for ^1H, 100.47 MHz for ^{13}C, 376.42 MHz for ^{19}F) or Bruker Avance 500 FT NMR (499.42 MHz for ^1H, 125.60 MHz for ^{13}C) spectrometer at room temperature. Chemical shifts are given in ppm and are referenced to residual ^1H and ^{13}C solvent signals. The ^{19}F NMR spectrum of [$^n Bu_4N$][**2**-μ_2-F] was referenced using C_6F_6 as a secondary external standard set at -161.64 ppm *vs*. $CFCl_3$.[3] Elemental analyses were performed by Atlantic Microlab (Norcross, GA). Electrospray ionization mass spectra were recorded on Applied Biosystems PE SCIEX QSTAR.

1.2 Single crystal X-ray diffraction measurements

The crystallographic measurements were performed at 100 K, 110 K, or 296 K using a Bruker D8 Quest (Mo source, λ = 0.71073 Å) or a Bruker APEX 22 (Mo source, λ = 0.71073 Å) diffractometer equipped with Photon III detectors, or a Rigaku XtaLAB Synergy-S diffractometer (Cu-Kα radiation, λ = 1.5418 Å) with a Dectris Eiger 2 detector. Semi-empirical absorption corrections were applied using the Bruker SADABS[4] within APEX3[5] or APEX4[6] using SCALE3 ABSPACK within Crysalis^{Pro}.[7] The structures were solved by direct methods with SHELXT[8] to locate all non-hydrogen atoms. Subsequent refinement using a difference map on F^2 with the SHEXL package[8] allowed for the location of the remaining non-hydrogen atoms which were refined anisotropically using the Olex2 interface.[9] H atoms were added in calculated positions using a riding model. Positional disorder was found to affect one of the DMSO solvent molecules in the solid-state structure of [$^n Bu_4N$][**2**-μ_2-F]. This disorder was modeled, leading to an improvement in the quality of the refinement. CCDC 2502484-2502487 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge *via* www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk

2. Experimental Procedure

2.1. Synthesis of 1, 2 and [^{n}Bu$_4$N][2-μ$_2$-F]

Synthesis of **1**: A solution of $PhSbCl_2$ (857.8 mg, 3.18 mmol) in THF (10 mL) was added dropwise to a suspension of 1,1′-dilithioferrocene·(tmeda) (1.04 g, 3.18 mmol) in mixture of Et_2O (15 mL) and THF (25 mL) at -78 °C. After stirring at this temperature for 30 min, the solution slowly warmed to room temperature and stirred for an additional 12 h. The solvent was removed *in vacuo* and CH_2Cl_2 (50 mL) was poured into the resulting sticky oil, which was washed with water (3 x 30 mL) and finally with brine (30 mL). The collected CH_2Cl_2 layer was dried over $MgSO_4$ and the solvent was removed *in vacuo* to afford a sticky orange oil. The residue was washed with pentane (100 mL) to afford a mixture of **1** (*syn* and *anti* isomers) and other unidentified compounds as a yellow-orange solid. The yellow-orange residue was subjected to flash column chromatography using 100-200 mesh silica gel and an eluent of hexanes/CH_2Cl_2 (7/3, *v/v*) to yield compound **1** (*syn* and *anti* isomers) in 6% yield (0.14 g, 0.183 mmol) as a yellow-orange solid. Preparative TLC was further performed using silica gel coated aluminum sheet to separate $\mathbf{1}_{syn}$ and $\mathbf{1}_{anti}$ using and eluent of hexanes/CH_2Cl_2 (8.5/1.5, *v/v*). This afforded pure $\mathbf{1}_{syn}$ (0.10 g, 4%, 0.131 mmol) as a yellow-orange solid. However, we were unsuccessful in isolating pure $\mathbf{1}_{anti}$ in an adequate amount required for further analysis except for single-crystal X-ray diffractometry. $\mathbf{1}_{anti}$ was inseparably contaminated with some unidentified products. Single crystals of $\mathbf{1}_{syn}$ and $\mathbf{1}_{anti}$ were obtained as yellowish-orange blocks by diffusing pentane into a CH_2Cl_2 solution at ambient temperature from the mixture of $\mathbf{1}_{syn}$ and $\mathbf{1}_{anti}$.

$\mathbf{1}_{syn}$: **^{1}H NMR** (400 MHz, $CDCl_3$, ppm): δ 7.23-7.22 (m, 4H, $H_{\text{Sb-phenyl}}$), 7.12-7.10 (m, 6H, $H_{\text{Sb-phenyl}}$), 4.67 (br, 4H, H_{Cp}), 4.51 (br, 8H, H_{Cp}), 4.45 (br, 4H, H_{Cp}). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, ppm): δ 141.9, 134.6, 128.3, 127.8, 75.7, 75.3, 71.6, 71.1, 70.8. **HRMS** (ESI-TOFMS, positive): *m/z* [M], calcd. for $[C_{32}H_{26}Sb_2Fe_2]^+$: 765.8808; found 765.8800.

Synthesis of 2: Under ambient conditions, a CH_2Cl_2 solution (5 mL) of *o*-chloranil (33.3 mg, 0.135 mmol) was added dropwise to a stirring CH_2Cl_2 solution of a mixture of isomers of **1** (50 mg, 6.5

× 10^{-2} mmol) in a vial at ambient temperature. After stirring for 2 h, the solvent was removed *in vacuo* and the resulting material was washed with pentane (70 mL) to obtain an orange solid as pure **2** in 80% yield (65 mg, 5.2 x 10^{-2} mmol). Single crystals of **2** were obtained as yellowish-orange blocks by slow evaporation of a CH_2Cl_2 solution at room temperature.

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.51-7.48 (m, 4H, $H_{\text{Sb-phenyl}}$), 7.45-7.41 (m, 2H, $H_{\text{Sb-phenyl}}$), 7.37-7.34 (m, 4H, $H_{\text{Sb-phenyl}}$), 5.06 (br, 4H, H_{Cp}), 5.03 (br, 4H, H_{Cp}), 4.77 (br, 4H, H_{Cp}), 4.52 (br, 4H, H_{Cp}). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$, ppm): δ 144.6, 136.6, 134.5, 129.7, 120.7, 116.3, 75.4, 74.9, 73.9, 73.7. **Elemental analysis:** calcd. (%) for $C_{44}H_{26}Cl_8Fe_2O_4Sb_2$-$CH_2Cl_2$: C, 40.26; H, 2.10; found C, 39.62; H, 1.88. The observed deviation from the calculated percentages suggests contamination by excess CH_2Cl_2, which is supported by integration of the ^{1}H NMR spectrum. **HRMS** (ESI-TOFMS, negative): *m/z* $[M+OH]^-$, calcd. for $C_{44}H_{27}Sb_2Fe_2O_5Cl_8$: 1274.6092; found 1274.6070.

Synthesis of [^{n}Bu$_4$N][2-μ$_2$-F]: Under ambient conditions, a solution of TBAT (22 mg, 4.1 x 10^{-2} mmol) in CH_2Cl_2 (2 mL) was slowly added to a solution of **2** (50 mg, 4.0 x 10^{-2} mmol) in CH_2Cl_2 (2 mL). After stirring for 2 h, the resulting solution was brought to dryness under vacuum, affording a light-yellow solid which was washed with pentane (100 mL). This procedure afforded [^{n}Bu$_4$N][**2**-μ$_2$-F] in 80% yield (49 mg, 3.2 x 10^{-2} mmol). Single crystals of [^{n}Bu$_4$N][**2**-μ$_2$-F] as pale-yellow blocks were obtained from DMSO upon diffusion of pentane.

^{1}H NMR (400 MHz, CD_2Cl_2, ppm): δ 7.22-7.20 (m, 4H, $H_{\text{Sb-phenyl}}$), 7.08-7.06 (m, 6H, $H_{\text{Sb-phenyl}}$), 5.31 (br, 4H, H_{Cp}, overlaps with the solvent resonance), 4.80 (br, 4H, H_{Cp}), 4.57-4.56 (br, 4H, H_{Cp}), 4.45 (br, 4H, H_{Cp}), 2.87-2.83 (m, 8H, H_{TBA}), 1.44 (m, 8H, H_{TBA}), 1.35-1.29 (m, 8H, H_{TBA}), 0.99-0.95 (t, J = 7.4 Hz, 12H, H_{TBA}). **^{13}C{^{1}H} NMR** (126 MHz, CD_2Cl_2, ppm): δ 149.6, 146.9, 132.9, 128.9, 128.4, 117.8, 115.3, 89.9, 76.2, 75.0, 70.9, 70.1, 59.4, 24.2, 20.1, 13.7. **^{19}F NMR** (469.86 MHz, CD_2Cl_2, ppm): δ = -32.00 (s). **Elemental analysis:** calcd. (%) for $C_{60}H_{62}NSb_2Fe_2O_4Cl_8F$: C, 47.44; H, 4.11; found C, 46.88; H, 4.05. **HRMS** (ESI-TOFMS, negative): *m/z* $[M]^-$, calcd. for $C_{44}H_{26}Sb_2Fe_2O_4Cl_8F$: 1276.6038; found 1276.6071.

2.2. NMR and mass spectra

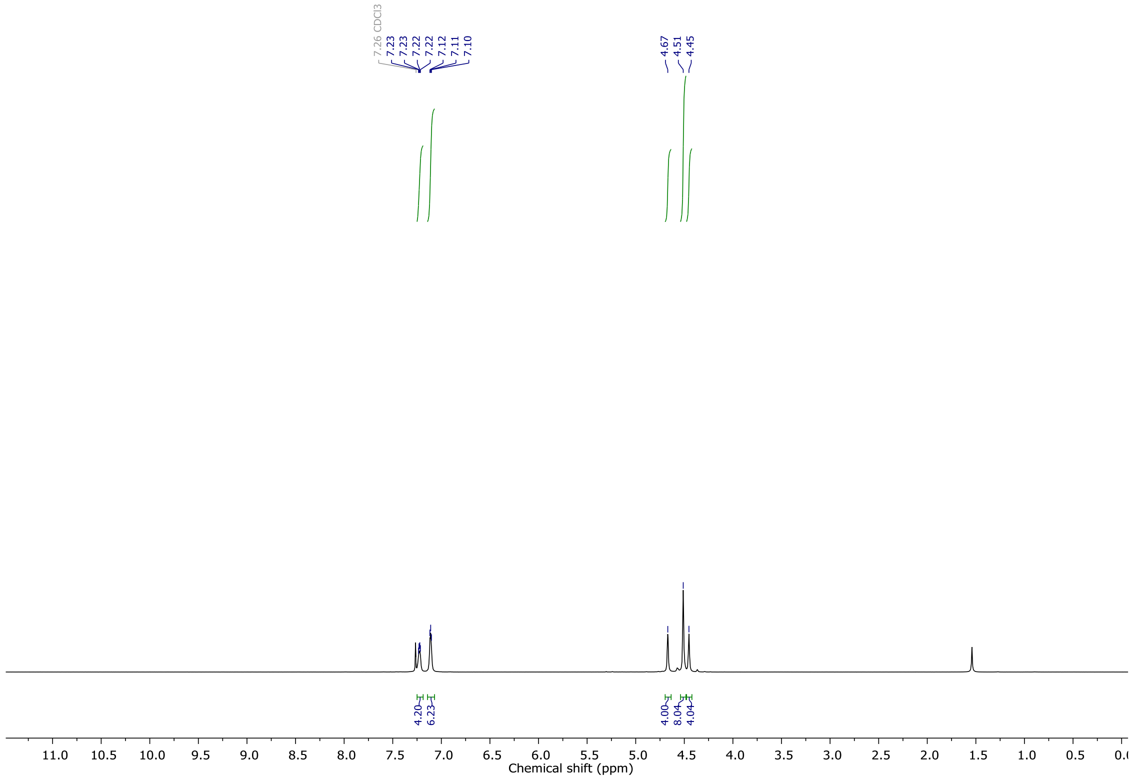


Fig. S1. [1]H NMR spectrum of $\mathbf{1}_{syn}$ in $CDCl_3$.

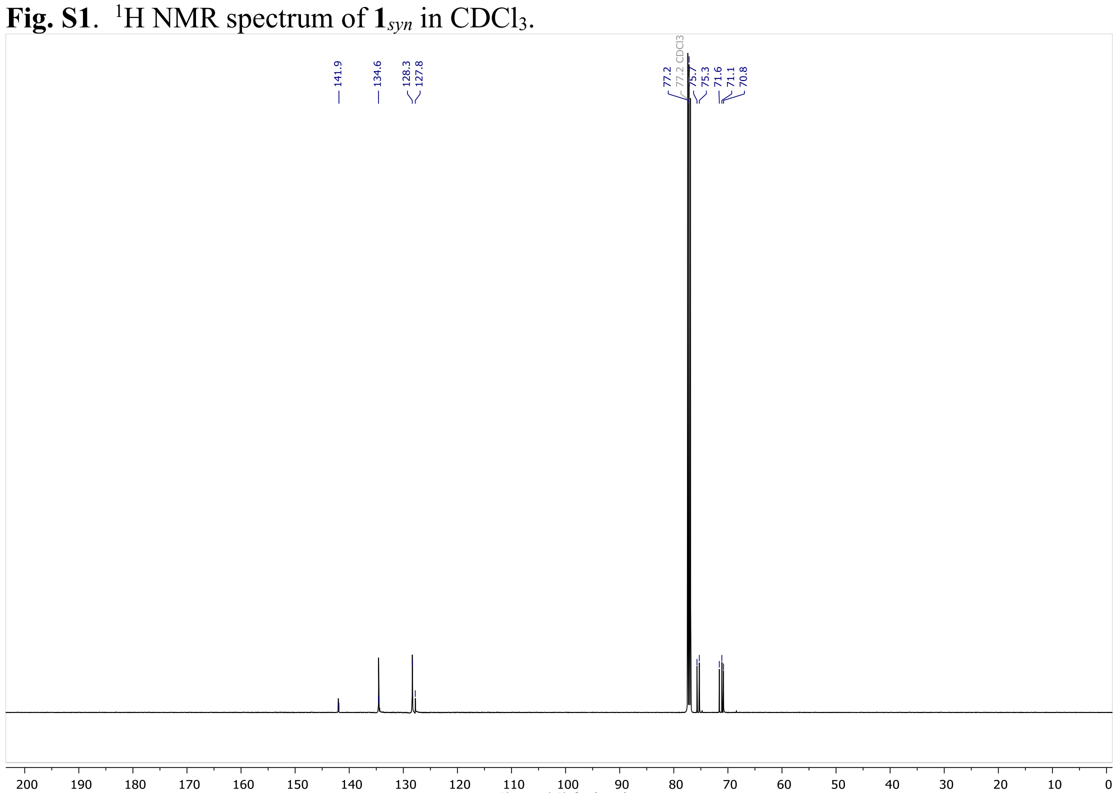


Fig. S2. [13]C{[1]H} NMR spectrum of $\mathbf{1}_{syn}$ in $CDCl_3$.

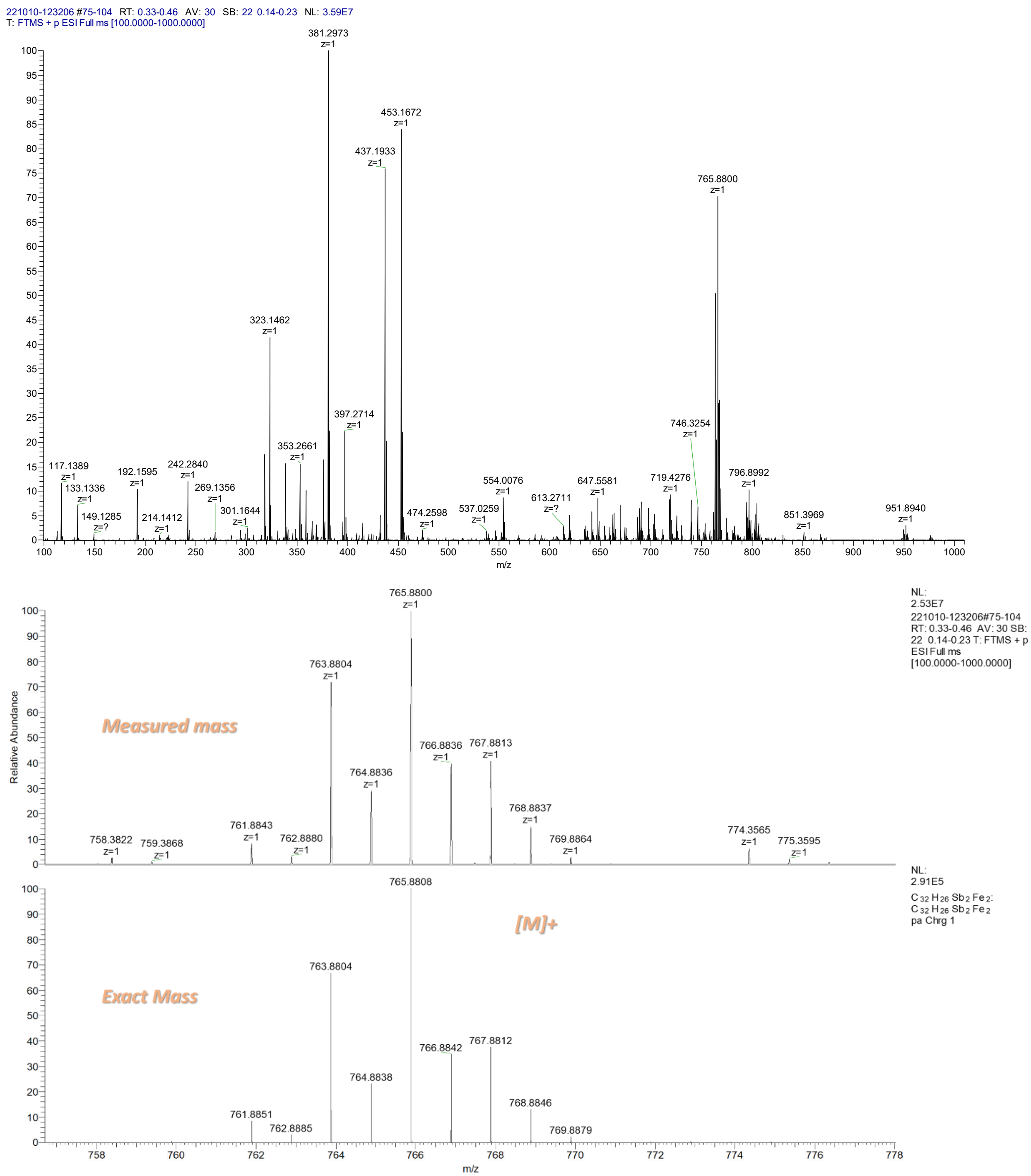


Fig. S3. HRMS of $\mathbf{1}_{syn}$.

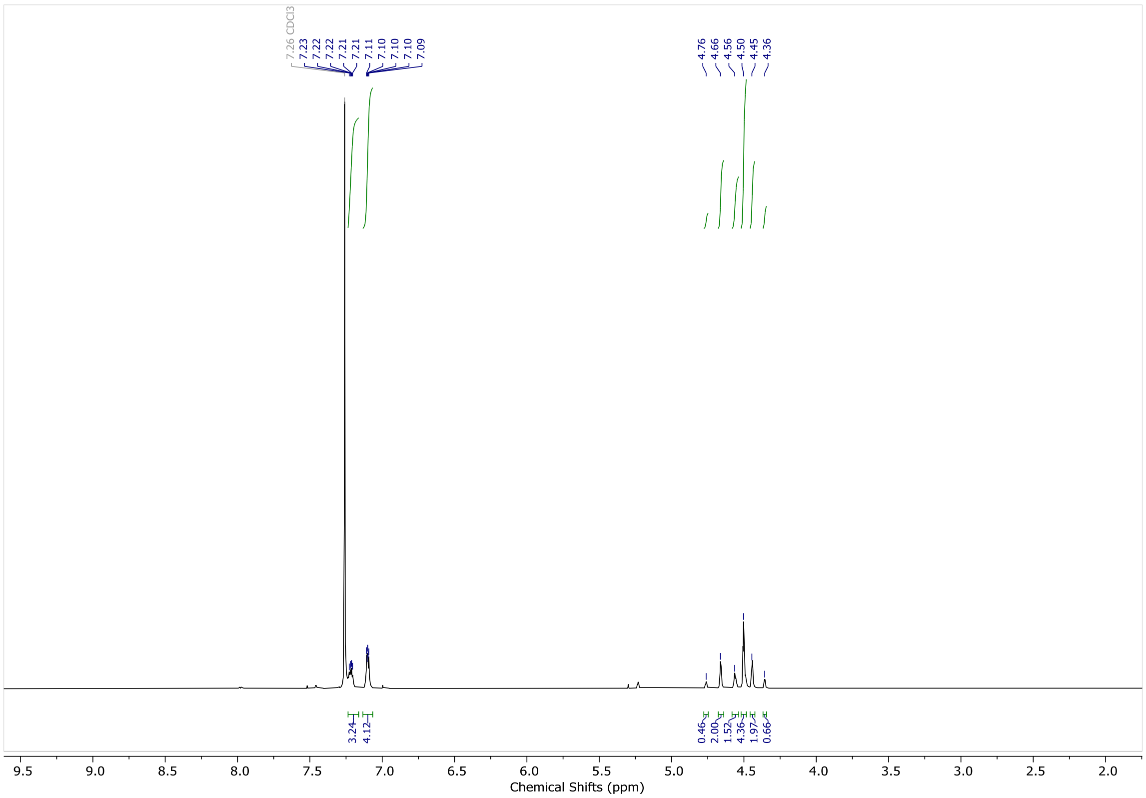


Fig. S4. Representative [1]H NMR spectrum of the mixture of $\mathbf{1}_{syn}$ and $\mathbf{1}_{anti}$ in $CDCl_3$.

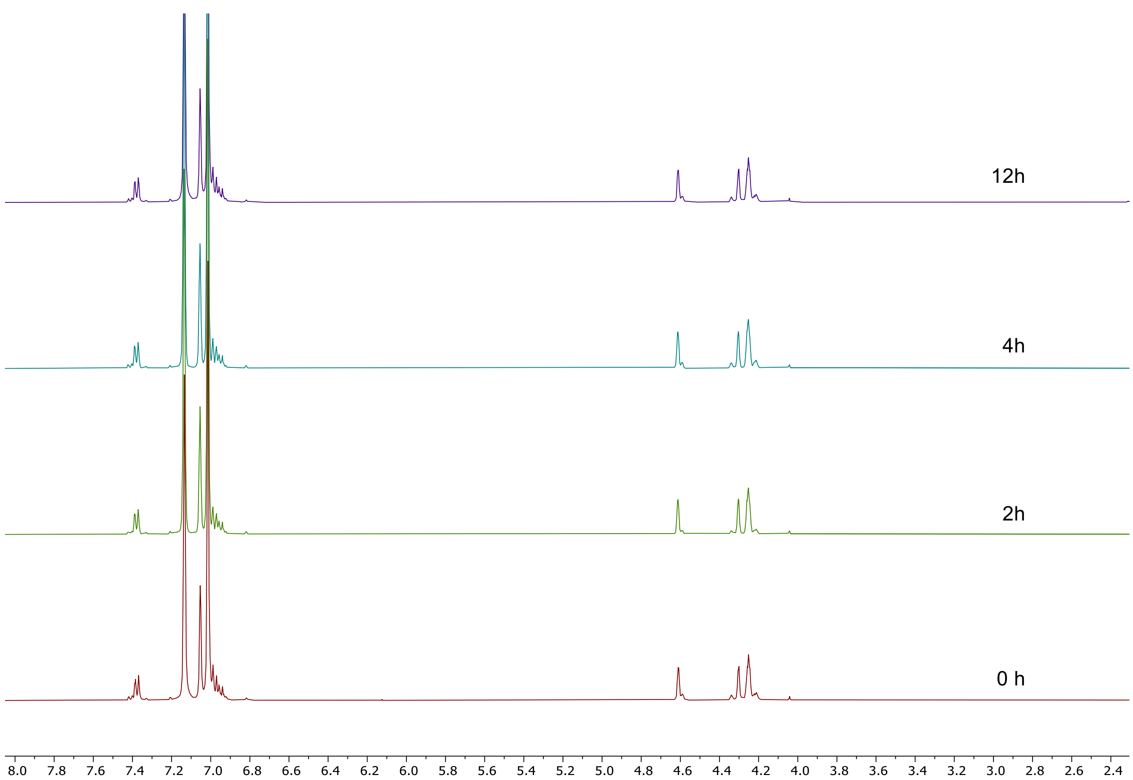


Fig. S5: [1]H NMR of $\mathbf{1}_{syn}$ (mixed with 10% $\mathbf{1}_{anti}$) in toluene-d_8 at 100 °C at different time intervals.

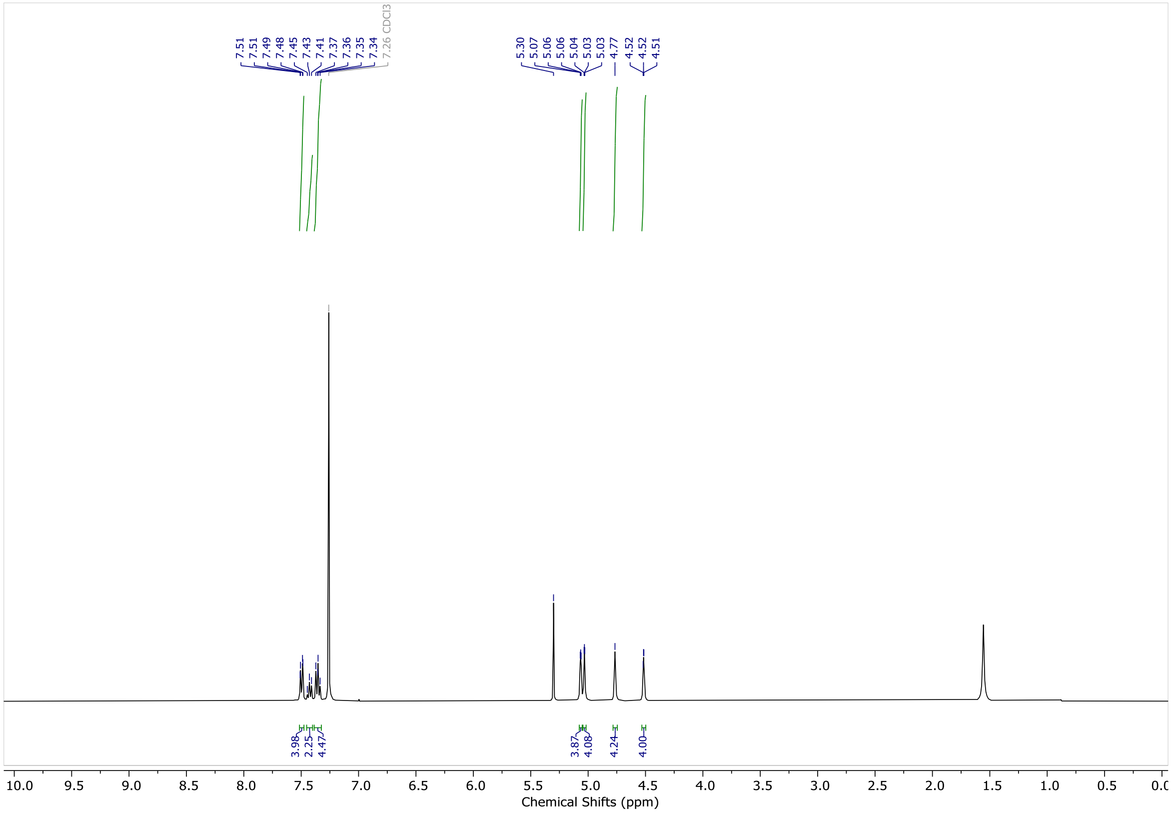


Fig. S6. [1]H NMR spectrum of **2** in $CDCl_3$. The resonance at 5.30 ppm corresponds to CH_2Cl_2.

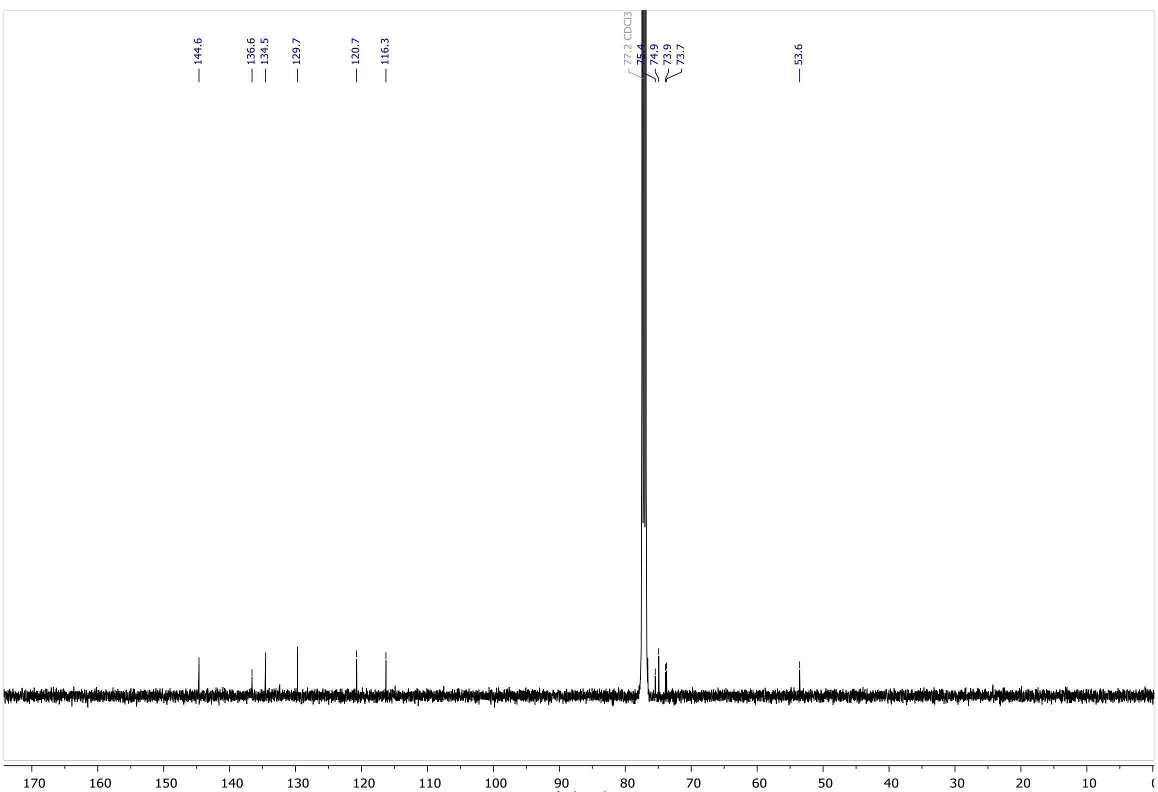


Fig. S7. [13]C{[1]H} NMR spectrum of **2** in $CDCl_3$.

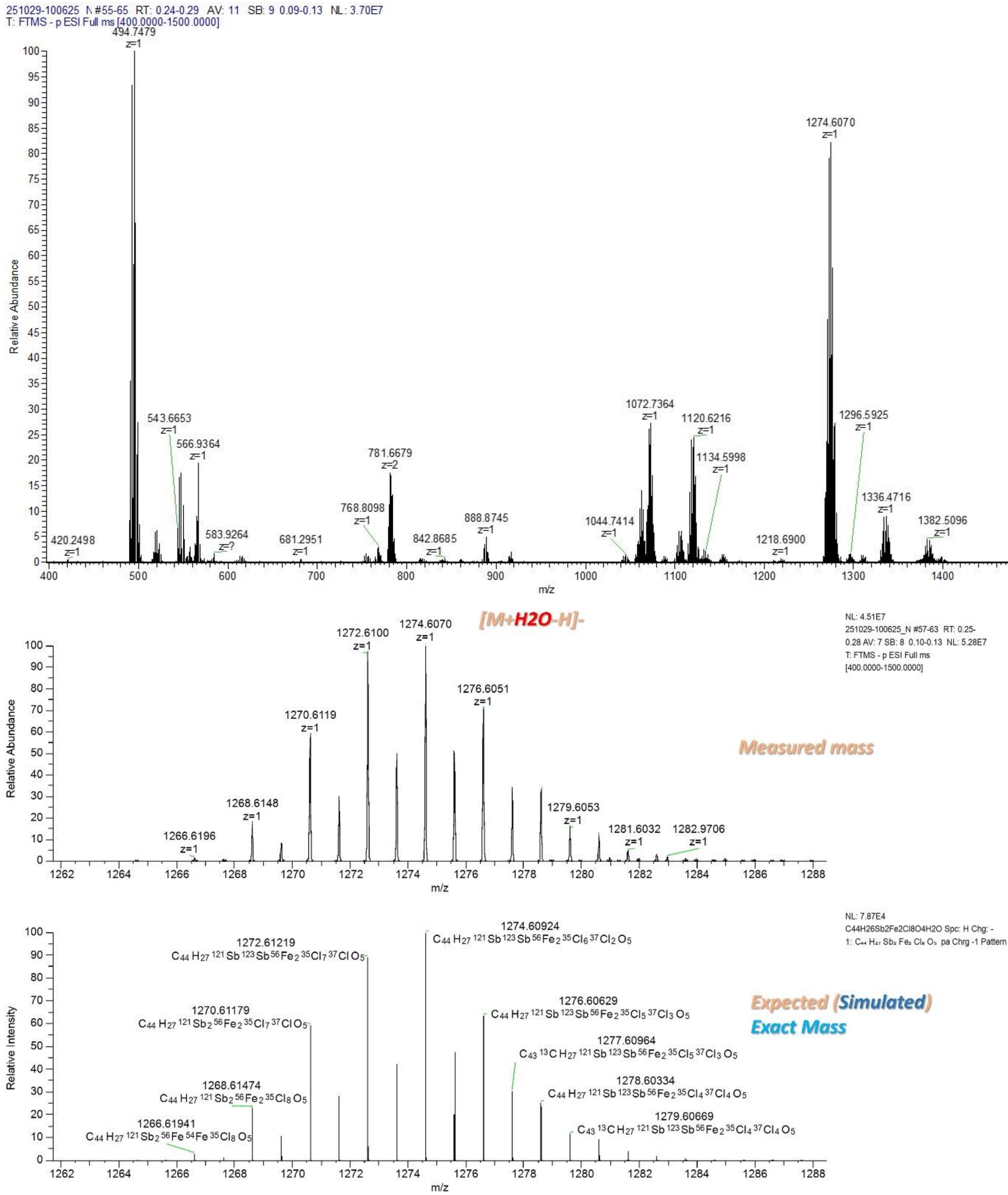


Fig. S8. HRMS of **2**.

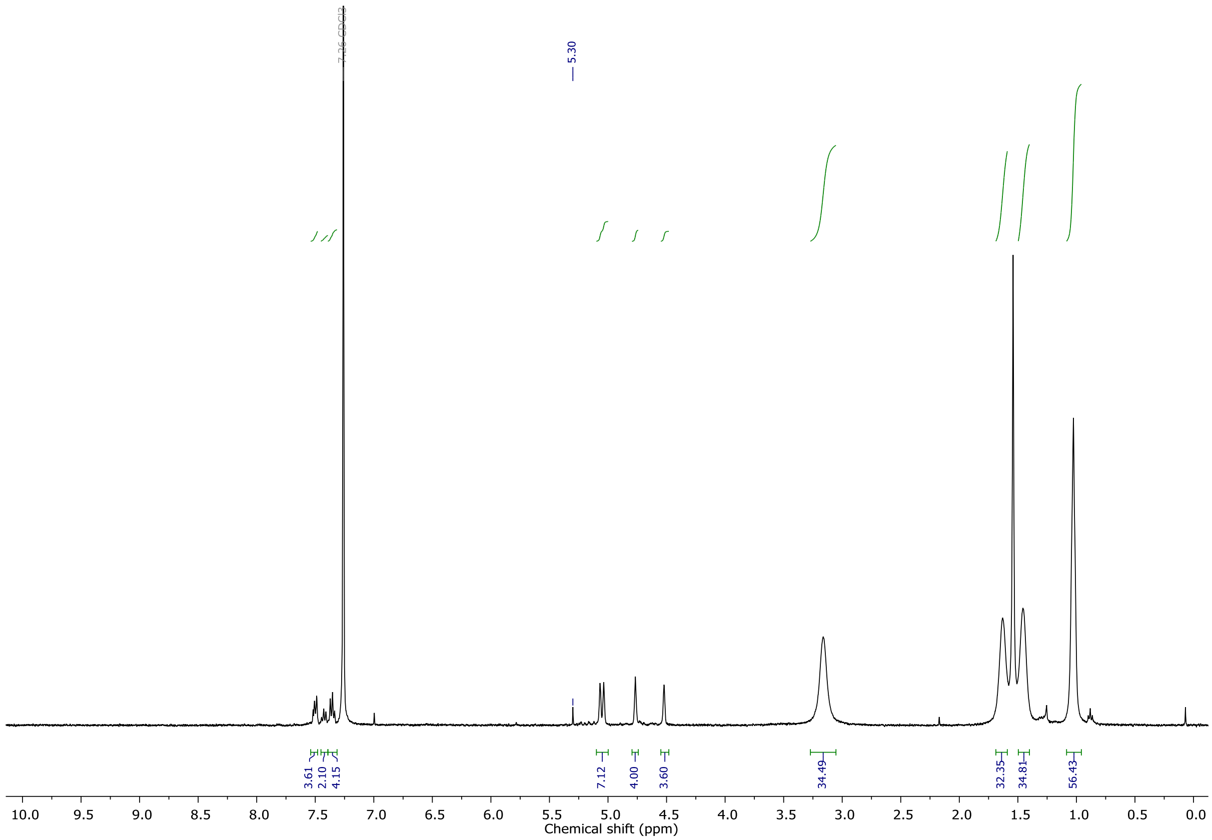


Fig. S9. [1]H NMR spectrum of **2** + [^{n}Bu$_4$N][PF$_6$] in CDCl$_3$.

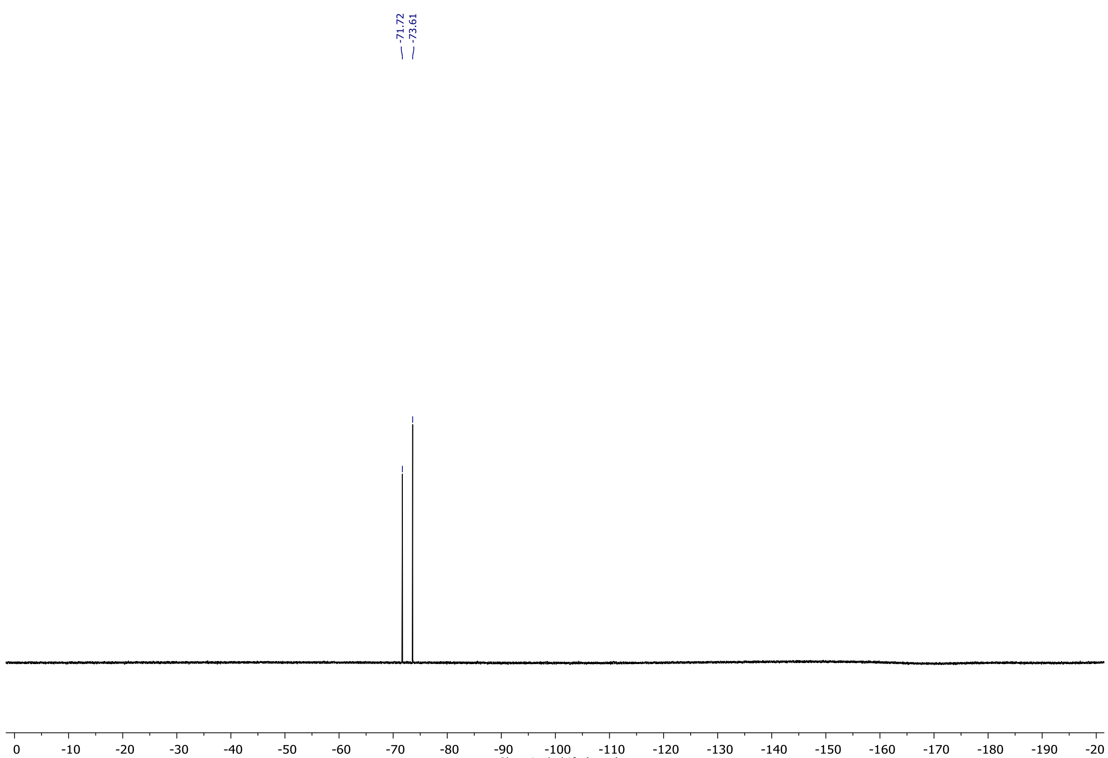


Fig. S10. [19]F NMR spectrum of **2** + [^{n}Bu$_4$N][PF$_6$] in CDCl$_3$.

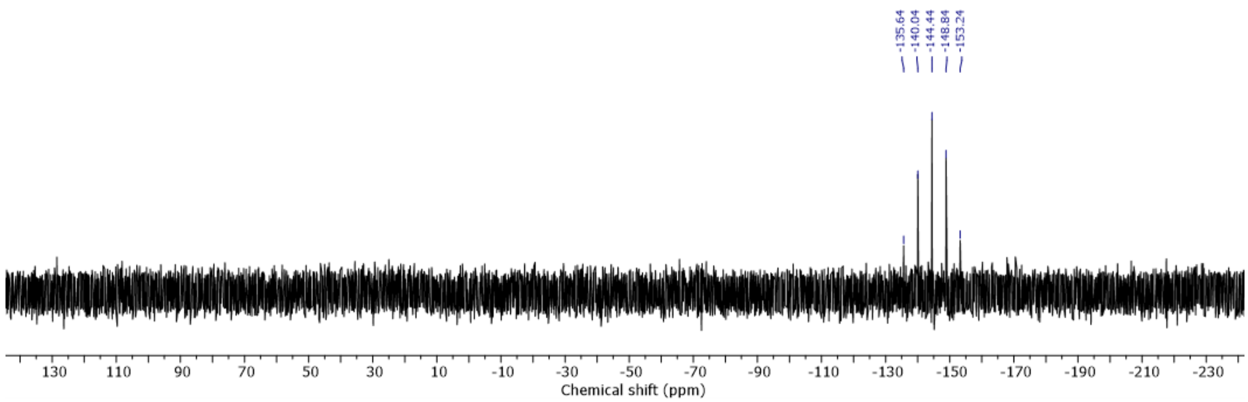


Fig. S11. ^{31}P NMR spectrum of **2** + [$^{n}Bu_4N$][PF_6] in $CDCl_3$.

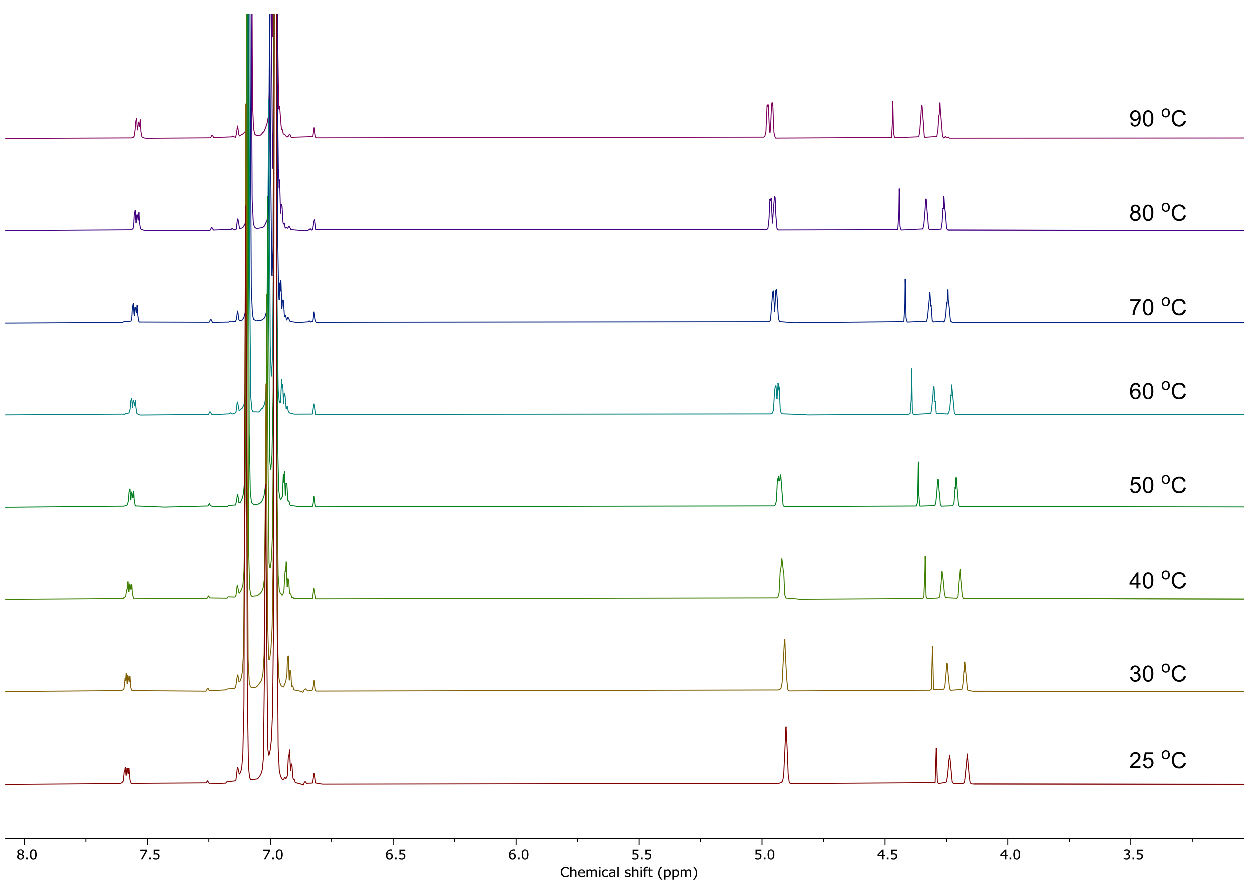


Fig S12. Variable temperature ^1H NMR of **2** in toluene-d_8. The peak at 4.28 ppm is due to CH_2Cl_2 present in the molecule.

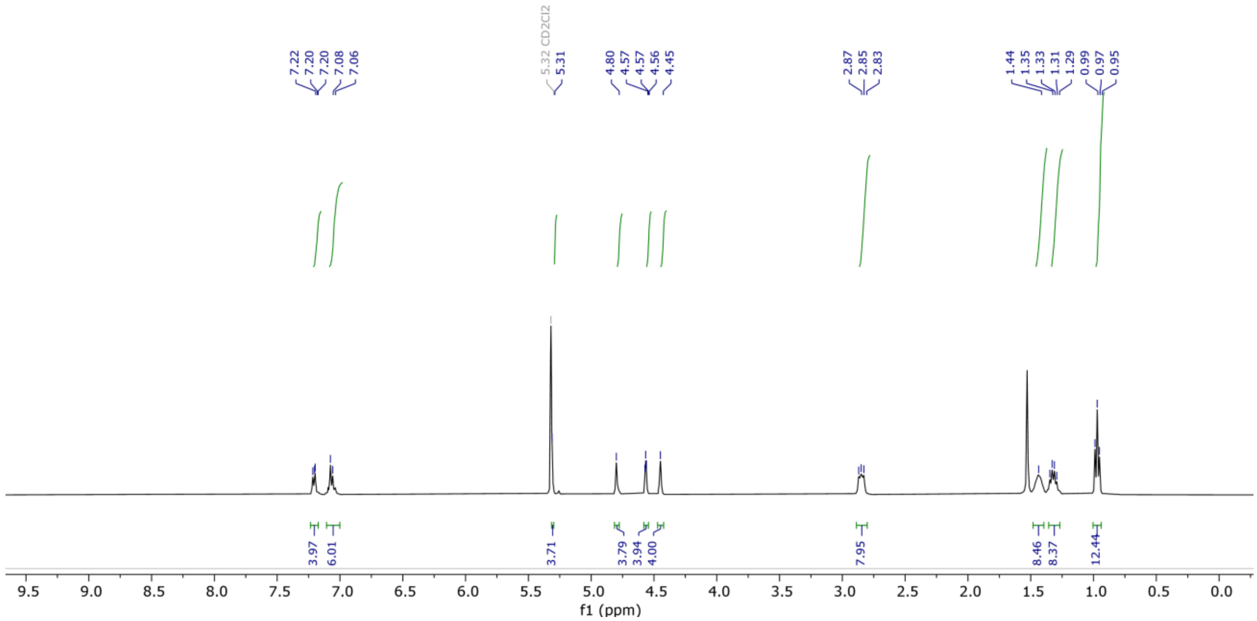


Fig. S13. ^{1}H NMR spectrum of [^{n}Bu$_4$N][**2**-μ$_2$-F] in CD_2Cl_2.

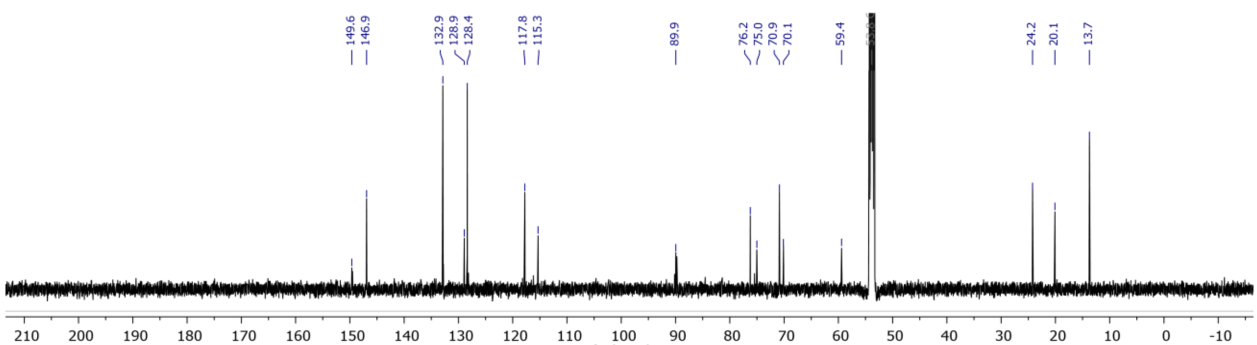


Fig. S14. ^{13}C{^{1}H} NMR spectrum of [^{n}Bu$_4$N][**2**-μ$_2$-F] in CD_2Cl_2.

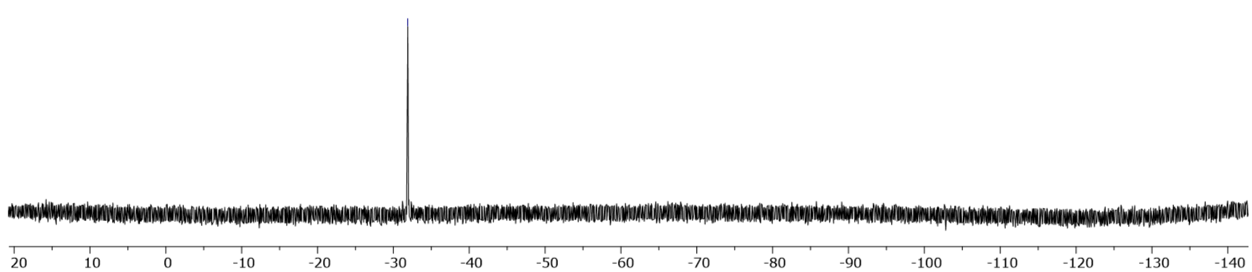


Fig. S15. ^{19}F NMR spectrum of [^{n}Bu$_4$N][**2**-μ$_2$-F] in CD_2Cl_2.

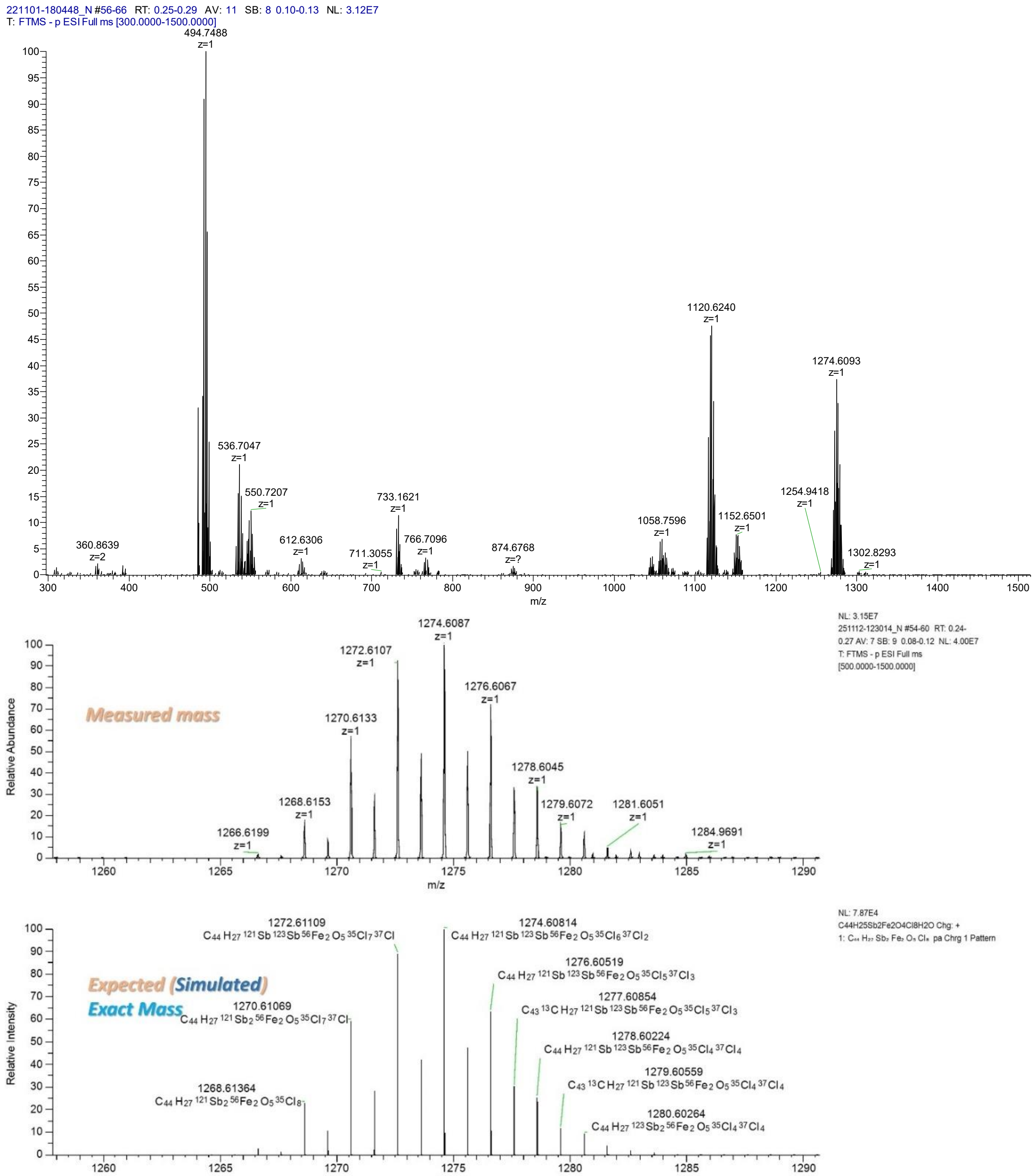


Fig. S16. HRMS spectrum of [^{n}Bu$_4$N][**2**-μ$_2$-F].

3. Cyclic Voltammetry

Cyclic voltammetry measurements were recorded with a CH Instrument (Model 660 D) electrochemical analyzer, using a glassy carbon working electrode, an Ag/AgCl reference electrode, a platinum wire auxiliary electrode, and a 1×10^{-4} M solution of **1**, **2**, and [^{n}Bu$_4$N][**2**-μ$_2$-

F] in degassed acetonitrile and tetrahydrofuran (1:1, *v*/*v*) with 0.1 M [$^{n}Bu_4N$][PF_6] as the supporting electrolyte. The voltammograms were collected at a scan rate of 0.1 V/s, referenced against Fc/Fc^+ in the same solvent, and were recorded at room temperature under N_2.

4. Computational details

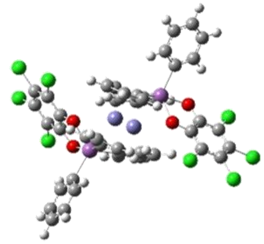
Density functional theory (DFT) calculations were performed with the Gaussian 16 program[10] using their crystal structure geometries as initial guesses. The structures were optimized using the B3LYP functional[11, 12] and the following mixed basis sets: aug-cc-pVTZ-PP[13-15] for Sb, aug-cc-pVTZ[16, 17] with CRENBL ECP[18] for Fe, 6-311G(d) for Cl,[19, 20] 6-31G(d') for F,[21, 22] and 6-31G for C, O & H.[23, 24] Frequency calculations were performed to confirm the absence of imaginary frequencies, reflecting that these structures are minima on the potential energy hypersurface. The enthalpies used to derive the FIA value were obtained by single-point calculations carried out at the optimized geometry with the B3LYP functional and the following mixed basis sets: aug-cc-pVTZ-PP for Sb, aug-cc-pVTZ with CRENBL ECP for Fe, def2-TZVPD for F,[25] and 6-311+g(2d,p) for all other elements. Diffuse functions were added for the F atom in single point calculations to align with the recent recommendations of Kaupp.[26] The *anti*-isomer of **2**, which corresponds to its solid-state geometry, was considered for the FIA calculation. For analysis of [**2**-μ_2-F]$^-$ at the anion binding geometry, the fluoride was removed and the resulting structure was subjected to a single point calculation at the aforementioned high level of theory. Orbitals were visualized using Avogadro[27] and the electrostatic potential map was visualized with GaussView.[28]

Table S1. FIA calculation details.

Compound	HF (Hartree)	H_{corr} (Hartree)	H	FIA (Hartree)	FIA (kJ/mol)
F^-	-99.9009819	0.002360	-99.8986219		
2	-6402.2410952	0.637869	-6401.6032262		
[**2**-μ_2-F]$^-$	-6502.2729635	0.639298	-6501.6336655	0.1318174	346.09

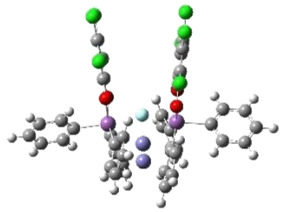
The reaction mechanism leading to the formation of [**2**-μ_2-F]$^-$ was computed using Gaussian 16. Gas-phase optimizations and frequency calculations were performed using the B3LYP functional and mixed basis sets: 6-31G(d) for C, H, O, F, Cl, 6-31g(d,p) for Fe and def2-TZVP for Sb. Frequency calculations were carried out to verify the nature of the stationary points: no imaginary frequency was found for the local minima and only one imaginary frequency was found for the transition states. The connectivity between each transition state and its two neighboring local minima was confirmed by intrinsic reaction coordinate (IRC) calculations.

Table S2. Optimized structure and XYZ coordinates of **2**.



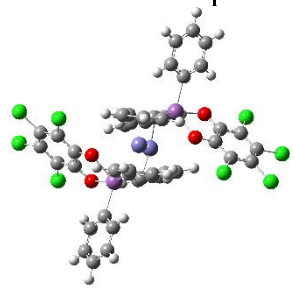
Sb	2.23466200	1.64242700	0.28605300
Sb	-2.23435500	-1.64241600	0.28548000
Fe	0.00022600	-0.00037400	3.10267300
Fe	-0.00027700	0.00041000	-2.10993500
Cl	4.49420700	-2.59128400	1.92417100
Cl	6.79975300	-3.61490200	-0.04257000
Cl	7.40133400	-2.00085500	-2.71006000
Cl	5.69550100	0.62154700	-3.38065800
Cl	-4.49502200	2.59015400	1.92486100
Cl	-6.80054900	3.61397200	-0.04179300
Cl	-7.40135200	2.00080500	-2.71002000
Cl	-5.69476000	-0.62088100	-3.38139400
O	3.13215000	-0.09863200	0.92819900
O	3.63475800	1.23353500	-1.26186300
O	-3.13213200	0.09831200	0.92807100
O	-3.63406500	-1.23311100	-1.26263400
C	1.14165900	1.49878200	2.10482800
C	1.76701300	1.12275000	3.35205700
H	2.74562700	0.67994500	3.45199800
C	0.85598200	1.41424600	4.41240200
H	1.02337100	1.21439500	5.46029900
C	-0.33797600	1.95905300	3.84019100
H	-1.23090100	2.24186000	4.37722500
C	-0.16957600	2.01553300	2.42384100
H	-0.90952000	2.38676500	1.73367700
C	0.33806000	-1.96003800	3.83970300
H	1.23087600	-2.24312100	4.37677100
C	-0.85588400	-1.41516200	4.41187400
H	-1.02337300	-1.21552500	5.45979800
C	-1.76670600	-1.12323500	3.35146300
H	-2.74524000	-0.68025400	3.45137900
C	-1.14122700	-1.49906500	2.10422000
C	0.16985900	-2.01613700	2.42331200
H	0.90982600	-2.38736900	1.73316500
C	0.78395600	1.72710800	-1.23004700
C	-0.65629700	1.71399500	-1.09323000
H	-1.22080400	1.69023700	-0.17575900
C	-1.21894200	1.71911100	-2.40787600
H	-2.27278700	1.69006700	-2.64062300
C	-0.14685800	1.72371300	-3.35541100
H	-0.25326800	1.69489100	-4.42959500
C	1.08921200	1.72391300	-2.64358500
H	2.08063800	1.70053000	-3.06496600
C	0.65666900	-1.71284500	-1.09348700
H	1.22099700	-1.68890800	-0.17590900
C	-0.78353600	-1.72721000	-1.23052300
C	-1.08862200	-1.72389900	-2.64407700
H	-2.08000700	-1.70122700	-3.06559000
C	0.14753400	-1.72252500	-3.35574500
H	0.25403400	-1.69345600	-4.42991300
C	1.21949800	-1.71720500	-2.40806900
H	2.27334600	-1.68728000	-2.64068700
C	3.22074500	3.50145800	0.64413900
C	4.19196600	3.98871700	-0.24959800
H	4.48095800	3.39728500	-1.10952000
C	4.78433000	5.23461600	-0.01358100
H	5.53411400	5.60994400	-0.70247800
C	4.41479100	5.99292700	1.10401500
H	4.87824700	6.95803300	1.28181900
C	3.44989500	5.50679900	1.99340500
H	3.16393200	6.09129100	2.86184800
C	2.85026200	4.26177800	1.76824400
H	2.10896600	3.88957000	2.46655400
C	-3.22098400	-3.50112700	0.64369400
C	-4.19242900	-3.98804200	-0.24997900
H	-4.48123600	-3.39653900	-1.10991400
C	-4.78527600	-5.23370800	-0.01390300
H	-5.53524300	-5.60874900	-0.70275800
C	-4.41598300	-5.99212600	1.10369100
H	-4.87979000	-6.95705400	1.28154900
C	-3.45084000	-5.50634800	1.99301700
H	-3.16507000	-6.09093300	2.86146100
C	-2.85073400	-4.26157600	1.76779800
H	-2.10925100	-3.88964000	2.46605000
C	4.14368300	-0.58776300	0.13332400
C	4.40688800	0.13546200	-1.04927200
C	5.40548200	-0.30143700	-1.92154400
C	6.14775000	-1.46021000	-1.61349000
C	5.88230900	-2.17580200	-0.43336200
C	4.86951000	-1.73339600	0.44367400
C	-4.14368900	0.58747900	0.13323400
C	-4.40653400	-0.13534600	-1.04968300
C	-5.40516400	0.30160200	-1.92190100
C	-6.14777400	1.46005200	-1.61346700
C	-5.88268600	2.17525200	-0.43302800
C	-4.86988800	1.73277500	0.44397400

Table S3. Optimized structure and XYZ coordinates of [**2**-μ_2-F]$^-$.



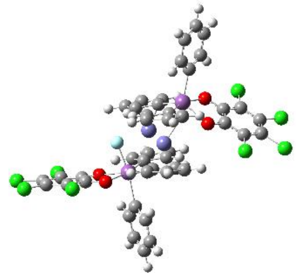
Sb	-1.06623600	-2.12358500	-0.31297100
Sb	-1.07299200	2.12024100	0.31302900
Fe	-2.95889400	0.39419600	-2.56099200
Fe	-2.95735300	-0.40350600	2.56125800
Cl	2.24055600	-2.99192100	3.45357300
Cl	3.41891700	2.20749800	2.70058900
Cl	2.23093700	2.99869000	-3.45369900
Cl	5.25177900	-3.21993900	2.39318000
Cl	5.83884600	2.83917100	0.70398100
Cl	3.42591200	-2.19653000	-2.70067400
Cl	5.84781100	-2.82106900	-0.70421200
Cl	5.24149200	3.23595500	-2.39343800
F	-0.56600400	-0.00062700	0.00007500
O	0.27691500	-2.39150800	1.26645000
O	0.76397000	2.06684900	1.31134600
O	0.26924400	2.39250200	-1.26644100
O	0.77056700	-2.06419900	-1.31133800
C	-1.97362400	-1.43105400	-2.10684400
C	1.56773200	2.48995800	-0.87621900
C	-3.46974500	1.17807800	3.87319200
H	-4.37392200	1.19585700	4.46445800
C	-1.29620600	4.24145700	0.71356900
C	-3.93158600	-1.50839400	1.03395900
H	-4.35943700	-1.09075200	0.13691200
C	-3.46545400	-1.18896400	-3.87337100
H	-4.36941100	-1.20987900	-4.46487100
C	-2.57069600	-1.96037700	1.18515600
C	1.83408500	2.31259400	0.50642200
C	3.93451300	2.87254300	-1.27555800
C	-2.43200400	2.42959700	-2.53797800
H	-1.51652000	2.81020400	-2.96220700
C	-3.32746700	1.68642800	2.54228700
H	-4.09387000	2.19303100	1.97422900
C	-1.28255200	-4.24543600	-0.71364600
C	3.14867500	-2.40642400	-0.98172300
C	4.19809900	2.69715600	0.09069400
C	-4.61667200	1.69289400	-2.27833300
H	-5.64045400	1.42095500	-2.49151100
C	-2.57708800	1.95231600	-1.18503000
C	-2.17592400	-5.04309800	0.02407900
H	-2.74811800	-4.60859100	0.83756000
C	1.84146400	-2.30672600	-0.50647700
C	-2.19214400	5.03616600	-0.02424500
H	-2.76283800	4.59978600	-0.83775000
C	-2.33090400	-6.40325100	-0.27624500
H	-3.02238100	-7.00812200	0.30404300
C	3.14100300	2.41630600	0.98160700
C	-0.54778000	-4.83572300	-1.75966500
H	0.14664900	-4.23185200	-2.33436700
C	-1.29551600	-0.74974900	-3.17647900
H	-0.27328500	-0.40750300	-3.14300200
C	-3.68922500	2.27128400	-3.20348700
H	-3.88946900	2.50230000	-4.23968000
C	-3.93654200	1.49606500	-1.03368300
H	-4.36310700	1.07715000	-0.13662400
C	-2.21536600	-0.60707200	-4.26249000
H	-2.01351700	-0.10898900	-5.19945000
C	-0.70418700	-6.19514300	-2.05758500
H	-0.12843100	-6.63889300	-2.86491700
C	-2.42396900	-2.43730800	2.53803200
H	-1.50724900	-2.81509500	2.96210700
C	2.62182300	-2.75999000	1.75594700
C	-1.97835000	1.42509000	2.10695700
C	4.20665300	-2.68412200	-0.09086300
C	-1.61831700	6.97614300	1.31710000
H	-1.74062400	8.03051700	1.54849800
C	1.57571700	-2.48500500	0.87615100
C	-1.29808600	0.74645100	3.17694000
H	-0.27465200	0.40777600	3.14380200
C	-3.68160400	-2.28298400	3.20368700
H	-3.88098200	-2.51470700	4.23988900
C	-4.61095700	-1.70745100	2.27866900
H	-5.63555800	-1.43870300	2.49197500
C	-1.59558100	-6.98116200	-1.31720300
H	-1.71437500	-8.03593600	-1.54861200
C	-2.21769100	0.60071700	4.26274900
H	-2.01434000	0.10357700	5.19988300
C	3.94365800	-2.86041400	1.27538100
C	2.61298000	2.76805200	-1.75607200
C	-0.72438700	6.19307500	2.05754900
H	-0.15015600	6.63872500	2.86492100
C	-0.56347300	4.83417400	1.75963600
H	0.13298100	4.23263100	2.33434200
C	-2.35164100	6.39580100	0.27608200
H	-3.04510700	6.99837400	-0.30422400
C	-3.32169900	-1.69711300	-2.54254600
H	-4.08640000	-2.20661500	-1.97477500

Table S4. XYZ coordinates of **2** obtained in the computational mechanistic studies.



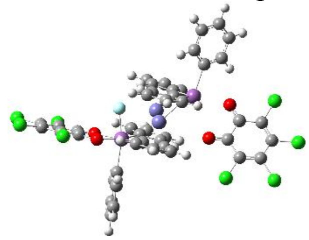
Sb	-2.178727	-1.629425	0.250825
Sb	2.178870	1.629891	0.249685
Fe	-0.000116	0.001324	3.083560
Fe	0.000254	-0.000969	-2.253180
Cl	-4.431008	2.557554	1.960732
Cl	-6.829136	3.532041	0.101965
Cl	-7.510585	1.906187	-2.528535
Cl	-5.789722	-0.674986	-3.263090
Cl	4.430475	-2.556302	1.962385
Cl	6.828253	-3.532589	0.104115
Cl	7.510013	-1.908568	-2.527433
Cl	5.789812	0.672610	-3.263513
O	-3.082101	0.119457	0.922755
O	-3.653947	-1.235056	-1.258944
O	3.082268	-0.118404	0.923040
O	3.654388	1.234609	-1.259545
C	-1.026316	-1.467084	2.061923
C	-1.655226	-1.180532	3.323950
H	-2.661882	-0.806875	3.451509
C	-0.716511	-1.439970	4.362988
H	-0.885352	-1.288435	5.421439
C	0.500188	-1.880172	3.761336
H	1.420815	-2.121846	4.276146
C	0.314293	-1.903197	2.350336
H	1.078513	-2.183271	1.640863
C	-0.500434	1.883352	3.759722
H	-1.421067	2.125523	4.274287
C	0.716230	1.443626	4.361808
H	0.885028	1.293018	5.420398
C	1.654994	1.183305	3.323029
H	2.661625	0.809705	3.450960
C	1.026158	1.468807	2.060722
C	-0.314452	1.905210	2.348713
H	-1.078675	2.184548	1.638952
C	-0.764905	-1.654847	-1.333439
C	0.671057	-1.654602	-1.248923
H	1.268518	-1.633208	-0.349928
C	1.188587	-1.658816	-2.576593
H	2.237289	-1.642261	-2.842248
C	0.087194	-1.659450	-3.483216
H	0.154326	-1.641412	-4.563246
C	-1.118796	-1.652025	-2.727940
H	-2.126751	-1.631000	-3.114571
C	-0.670722	1.653471	-1.250451
H	-1.268264	1.632900	-0.351490
C	0.765266	1.653667	-1.334806
C	1.119317	1.649671	-2.729269
H	2.127329	1.628390	-3.115740
C	-0.086587	1.656384	-3.484682
H	-0.153620	1.637382	-4.564702
C	-1.188092	1.656497	-2.578186
H	-2.236753	1.639659	-2.843986
C	-3.110859	-3.534773	0.621207
C	-4.148365	-3.993450	-0.201257
H	-4.511229	-3.375873	-1.014651
C	-4.709850	-5.248918	0.040044
H	-5.515776	-5.605766	-0.595335
C	-4.241423	-6.040740	1.090909
H	-4.683173	-7.016462	1.274171
C	-3.207028	-5.579775	1.907370
H	-2.840933	-6.193057	2.726133
C	-2.638652	-4.324740	1.677473
H	-1.837984	-3.973712	2.320561
C	3.111034	3.535403	0.619158
C	4.149160	3.993310	-0.202947
H	4.512316	3.375162	-1.015772
C	4.710817	5.248787	0.037926
H	5.517240	5.605023	-0.597165
C	4.241915	6.041393	1.087983
H	4.683798	7.017117	1.270919
C	3.206859	5.581216	1.904056
H	2.840370	6.195127	2.722171
C	2.638328	4.326174	1.674606
H	1.837160	3.975764	2.317405
C	-4.109513	0.562081	0.170484
C	-4.407467	-0.168639	-1.002818
C	-5.456162	0.254181	-1.825278
C	-6.208795	1.396132	-1.490275
C	-5.908423	2.116965	-0.325359
C	-4.851450	1.692803	0.504036
C	4.109541	-0.561749	0.171009
C	4.407641	0.168141	-1.002774
C	5.456135	-0.255506	-1.825055
C	6.208472	-1.397461	-1.489382
C	5.907960	-2.117478	-0.324000
C	4.851149	-1.692504	0.505187

Table S5. XYZ coordinates of **Int-1** obtained in the computational mechanistic studies.



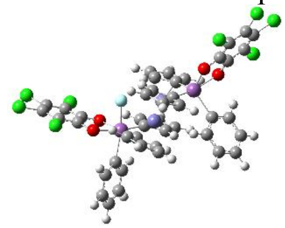
Sb	-2.589256	-1.560828	-0.050681
Sb	2.310096	0.846914	0.114658
Fe	-0.094056	-0.674565	2.788423
Fe	-0.304777	-0.075117	-2.636327
Cl	-4.506158	2.157669	2.805146
Cl	-7.013322	3.603154	1.470564
Cl	-7.974162	2.698182	-1.409975
Cl	-6.416400	0.357433	-2.915548
Cl	6.294179	-0.738690	2.841964
Cl	8.772906	-1.548037	1.007686
Cl	8.559664	-1.194947	-2.137614
Cl	5.869673	-0.038274	-3.399869
O	-3.326966	0.050175	1.064080
O	-4.127856	-0.703453	-1.319066
O	4.007765	0.333449	1.292958
O	3.826091	0.627341	-1.362974
C	-1.301071	-1.862032	1.637765
C	-1.800898	-1.776528	2.988106
H	-2.763849	-1.378663	3.276515
C	-0.796220	-2.277974	3.865830
H	-0.862109	-2.317683	4.945850
C	0.328993	-2.667231	3.076375
H	1.272987	-3.044791	3.447436
C	0.024688	-2.418296	1.707304
H	0.725018	-2.536131	0.895782
C	-0.473590	1.183808	3.577698
H	-1.399867	1.466539	4.060771
C	0.671649	0.602140	4.201167
H	0.774968	0.367837	5.253540
C	1.643601	0.348607	3.187038
H	2.620978	-0.092779	3.324730
C	1.112822	0.771250	1.923559
C	-0.200460	1.290003	2.182304
H	-0.899192	1.679051	1.456829
C	-1.402323	-1.575985	-1.806859
C	-0.025366	-1.975845	-1.935352
H	0.679051	-2.176828	-1.144616
C	0.311813	-1.917955	-3.316604
H	1.291215	-2.127210	-3.726385
C	-0.837425	-1.485074	-4.045923
H	-0.888464	-1.320092	-5.114730
C	-1.899094	-1.264995	-3.124183
H	-2.898566	-0.927448	-3.351341
C	-0.458104	1.617181	-1.477845
H	-1.074324	1.722366	-0.595832
C	0.906396	1.172167	-1.517413
C	1.296271	1.177782	-2.898307
H	2.269829	0.878387	-3.260977
C	0.190735	1.614815	-3.689040
H	0.174914	1.701079	-4.768454
C	-0.900362	1.884437	-2.809275
H	-1.891554	2.212800	-3.094928
C	-3.788294	-3.350861	0.115443
C	-4.901731	-3.546586	-0.712613
H	-5.189781	-2.777678	-1.420768
C	-5.636143	-4.730436	-0.616165
H	-6.500538	-4.879192	-1.258356
C	-5.264564	-5.717218	0.299860
H	-5.839867	-6.636909	0.372073
C	-4.154260	-5.521882	1.123067
H	-3.861164	-6.286770	1.837638
C	-3.413938	-4.340132	1.034005
H	-2.554130	-4.195196	1.680475
C	2.821900	2.973644	0.306296
C	3.237988	3.699291	-0.817696
H	3.326495	3.203292	-1.779538
C	3.553805	5.056249	-0.710396
H	3.873676	5.607401	-1.592176
C	3.465047	5.701684	0.524999
H	3.711720	6.757795	0.609165
C	3.063629	4.982842	1.652288
H	2.999210	5.475850	2.620000
C	2.745968	3.625565	1.542730
H	2.442163	3.077953	2.430511
C	-4.388989	0.682525	0.545272
C	-4.815878	0.270331	-0.743058
C	-5.919515	0.897278	-1.329610
C	-6.600675	1.928251	-0.654290
C	-6.176505	2.329504	0.618503
C	-5.066612	1.698324	1.216622
C	5.045599	-0.028257	0.553924
C	4.950258	0.130148	-0.865064
C	6.031997	-0.242734	-1.666900
C	7.216770	-0.757210	-1.102141
C	7.310431	-0.912236	0.283608
C	6.220371	-0.552277	1.101689
F	2.166116	-1.149840	-0.082317

Table S6. XYZ coordinates of **TS1** obtained in the computational mechanistic studies.



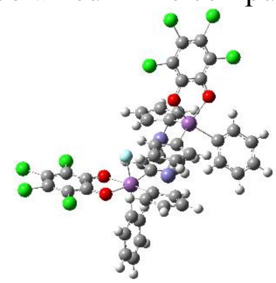
Sb	2.497849	1.654490	0.363281
Sb	-2.352171	-0.758081	-0.028912
Fe	-0.113635	0.581153	2.871956
Fe	0.300624	0.495656	-2.597006
Cl	4.144560	-3.750247	1.073509
Cl	7.293218	-4.190933	1.016215
Cl	9.159273	-2.063396	-0.293520
Cl	7.947378	0.581036	-1.569676
Cl	-6.413063	0.227411	2.903757
Cl	-9.003875	0.948501	1.194123
Cl	-8.842608	0.906122	-1.968605
Cl	-6.092318	0.143096	-3.386014
O	3.367338	-1.266134	-0.333089
O	4.993535	0.619299	-1.398075
O	-4.074813	-0.446952	1.219686
O	-3.938743	-0.483921	-1.455522
C	1.047907	2.001189	1.929570
C	1.438267	1.837469	3.306569
H	2.418763	1.535138	3.654836
C	0.319395	2.140920	4.138380
H	0.299594	2.096408	5.220167
C	-0.775850	2.480449	3.287523
H	-1.781305	2.727012	3.604025
C	-0.334964	2.391147	1.933488
H	-0.978682	2.505526	1.075884
C	0.464663	-1.327214	3.367857
H	1.413533	-1.598577	3.813259
C	-0.728061	-0.971256	4.066977
H	-0.846635	-0.920636	5.142340
C	-1.729487	-0.662522	3.097724
H	-2.743745	-0.345983	3.297185
C	-1.168036	-0.824749	1.786399
C	0.194096	-1.241857	1.968212
H	0.918938	-1.446311	1.192477
C	1.376055	1.855176	-1.466543
C	0.052083	2.342238	-1.735580
H	-0.725090	2.539204	-1.014482
C	-0.114689	2.428986	-3.149314
H	-1.019532	2.739993	-3.655980
C	1.092430	1.984641	-3.769114
H	1.272281	1.907462	-4.834245
C	2.007647	1.621711	-2.737321
H	3.008711	1.234832	-2.873780
C	0.358351	-1.377568	-1.738366
H	0.972227	-1.661691	-0.896972
C	-0.978479	-0.856844	-1.697256
C	-1.370070	-0.609000	-3.055333
H	-2.328474	-0.209940	-3.356961
C	-0.287765	-0.964732	-3.914709
H	-0.274263	-0.867303	-4.993302
C	0.784517	-1.436895	-3.098481
H	1.759242	-1.760447	-3.440703
C	3.349397	3.685797	0.349582
C	4.576616	3.893258	-0.294191
H	5.085641	3.063800	-0.780808
C	5.155227	5.165677	-0.321288
H	6.105621	5.315797	-0.828915
C	4.518183	6.238769	0.305143
H	4.970098	7.227936	0.288122
C	3.299447	6.036131	0.956684
H	2.797291	6.868142	1.445701
C	2.717394	4.765441	0.981054
H	1.767547	4.621275	1.488772
C	-2.810027	-2.906569	-0.031978
C	-2.893989	-3.607870	-1.240904
H	-2.740619	-3.087752	-2.182258
C	-3.178338	-4.976342	-1.249857
H	-3.238591	-5.509322	-2.196419
C	-3.388733	-5.656189	-0.048298
H	-3.610692	-6.721145	-0.054470
C	-3.317702	-4.961303	1.160846
H	-3.487049	-5.482528	2.100737
C	-3.033300	-3.592684	1.167725
H	-2.988522	-3.061582	2.114265
C	4.584139	-1.450175	-0.307688
C	5.493968	-0.400532	-0.921623
C	6.936366	-0.637741	-0.863003
C	7.445359	-1.779504	-0.299560
C	6.572919	-2.775642	0.311154
C	5.212981	-2.605084	0.336301
C	-5.156139	-0.132122	0.538921
C	-5.082607	-0.151665	-0.897310
C	-6.224397	0.176144	-1.641443
C	-7.434244	0.513748	-1.008008
C	-7.505776	0.532503	0.392327
C	-6.366893	0.213552	1.154108
F	-2.341876	1.242016	-0.064076

Table S7. XYZ coordinates of **Int-2** obtained in the computational mechanistic studies.



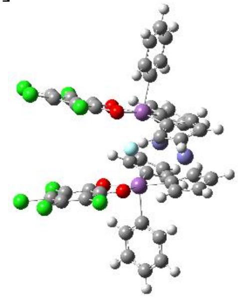
Sb	-2.797946	0.677392	0.186085
Fe	-0.104223	1.361340	-2.579391
Fe	0.151904	-0.305622	2.548708
Cl	-6.207189	-0.905972	-3.229721
Cl	-8.146716	-3.147672	-2.055298
Cl	-7.835194	-4.039899	0.972621
Cl	-5.588800	-2.677641	2.778631
O	4.467108	-0.255474	1.185040
O	-4.288515	0.131513	-1.228851
O	-4.026311	-0.621528	1.330262
C	1.532509	0.321594	-1.857851
C	1.899760	1.101196	-3.011690
H	2.672660	1.857488	-3.049574
C	1.100685	0.682464	-4.111439
H	1.128217	1.101690	-5.109215
C	0.235923	-0.356418	-3.657244
H	-0.524794	-0.858787	-4.240331
C	0.496975	-0.582709	-2.277885
H	-0.067332	-1.260368	-1.658503
C	-0.613854	3.359740	-2.613066
H	0.051398	4.178740	-2.857813
C	-1.411821	2.617003	-3.534933
H	-1.447785	2.762187	-4.607510
C	-2.130386	1.628857	-2.796916
H	-2.816812	0.896882	-3.199652
C	-1.786972	1.745485	-1.412277
C	-0.852204	2.825847	-1.310736
H	-0.410078	3.199433	-0.398443
C	1.662807	-0.944130	1.333893
C	0.489860	-1.754028	1.142686
H	-0.124472	-1.833192	0.261537
C	0.173924	-2.357459	2.391805
H	-0.679458	-2.997201	2.573834
C	1.135361	-1.930809	3.356966
H	1.151276	-2.202246	4.404788
C	2.057130	-1.059090	2.713954
H	2.919636	-0.589743	3.162807
C	-0.324870	1.647772	2.119219
H	0.165598	2.264756	1.380087
C	-1.469051	0.807523	1.905697
C	-1.746556	0.170614	3.161638
H	-2.548682	-0.535823	3.325078
C	-0.788407	0.610376	4.124859
H	-0.728806	0.286239	5.156407
C	0.097658	1.524724	3.478558
H	0.945950	2.025386	3.927589
C	-4.020932	2.409771	0.766766
C	-4.015052	2.909875	2.074175
H	-3.413544	2.429061	2.840450
C	-4.784740	4.027504	2.412545
H	-4.770752	4.403317	3.433529
C	-5.571020	4.655840	1.445475
H	-6.170282	5.524924	1.707990
C	-5.589166	4.158395	0.140371
H	-6.205746	4.637190	-0.617386
C	-4.821740	3.040169	-0.195601
H	-4.856115	2.649686	-1.208245
C	-5.097833	-0.813855	-0.768953
C	-4.957198	-1.216462	0.596147
C	-5.799007	-2.209908	1.103797
C	-6.787070	-2.810583	0.297809
C	-6.924256	-2.417634	-1.036553
C	-6.072604	-1.425081	-1.562134
F	-1.944656	-1.033091	-0.427816
Sb	2.750551	0.197947	-0.087104
C	3.127842	2.276830	0.377432
C	2.490138	3.272766	-0.372817
C	4.009883	2.631279	1.407781
C	2.730713	4.620131	-0.089424
H	1.801627	3.000268	-1.163600
C	4.237501	3.980634	1.688099
H	4.520707	1.859654	1.971263
C	3.601201	4.975114	0.941935
H	2.233243	5.388627	-0.675515
H	4.919596	4.252269	2.489687
H	3.784765	6.023526	1.162859
O	4.125492	-0.658723	-1.393174
C	5.312777	-0.995646	-0.864917
C	6.345772	-1.536199	-1.627461
C	5.489732	-0.771354	0.525485
C	7.576214	-1.868509	-1.023761
C	6.715161	-1.099057	1.115948
C	7.758511	-1.649067	0.346994
Cl	6.071393	-1.783522	-3.333102
Cl	8.861551	-2.549415	-1.991187
Cl	9.277485	-2.052377	1.110799
Cl	6.899668	-0.799058	2.828172

Table S8. XYZ coordinates of **TS2** obtained in the computational mechanistic studies.



Sb	-2.658169	-0.784794	-0.148129
Fe	-0.199823	-1.515527	2.808138
Fe	0.350739	-0.678963	-2.632970
Cl	-5.666301	1.875634	2.964330
Cl	-7.169910	4.251003	1.460042
Cl	-6.730331	4.639534	-1.657135
Cl	-4.793586	2.648403	-3.221179
O	4.800320	-0.551191	-0.268708
O	-3.988690	0.237396	1.158361
O	-3.617332	0.565785	-1.475658
C	1.542401	-0.706473	2.061402
C	1.812974	-1.469129	3.253575
H	2.481635	-2.316280	3.333587
C	1.059222	-0.899929	4.318741
H	1.026509	-1.267529	5.336595
C	0.327417	0.210717	3.800284
H	-0.374323	0.825211	4.349072
C	0.622755	0.335939	2.416497
H	0.166709	1.041704	1.738707
C	-0.962309	-3.420920	3.013642
H	-0.415304	-4.283869	3.372955
C	-1.695872	-2.492921	3.812379
H	-1.792578	-2.517435	4.890765
C	-2.249733	-1.506091	2.942419
H	-2.846842	-0.652903	3.233328
C	-1.866930	-1.808242	1.596577
C	-1.076150	-3.001506	1.654326
H	-0.647716	-3.521676	0.810242
C	1.876158	0.000436	-1.466592
C	0.880455	1.025011	-1.607751
H	0.264964	1.435923	-0.821622
C	0.749297	1.310367	-2.994871
H	0.044537	2.010748	-3.423448
C	1.661098	0.481180	-3.717444
H	1.783851	0.453644	-4.792643
C	2.362419	-0.330529	-2.780407
H	3.128402	-1.058447	-3.012051
C	-0.397123	-2.435079	-1.876616
H	0.025981	-2.978633	-1.044522
C	-1.399944	-1.409126	-1.808613
C	-1.613899	-0.958510	-3.154380
H	-2.305636	-0.176320	-3.435097
C	-0.759263	-1.694451	-4.029652
H	-0.679880	-1.561494	-5.101454
C	-0.001803	-2.609569	-3.237800
H	0.752852	-3.298341	-3.595829
C	-4.211935	-2.302846	-0.504629
C	-4.251235	-3.053131	-1.686076
H	-3.521380	-2.876381	-2.470844
C	-5.230819	-4.033153	-1.876145
H	-5.248567	-4.605587	-2.801320
C	-6.184004	-4.273284	-0.885368
H	-6.946641	-5.034872	-1.032773
C	-6.156181	-3.525522	0.293980
H	-6.899692	-3.700815	1.068647
C	-5.178564	-2.545055	0.481695
H	-5.175011	-1.957421	1.394509
C	-4.614211	1.242792	0.558638
C	-4.415506	1.417852	-0.846431
C	-5.066800	2.467256	-1.500835
C	-5.919156	3.345452	-0.801685
C	-6.112729	3.174689	0.572087
C	-5.452876	2.125796	1.243646
F	-1.463318	0.783043	0.235186
Sb	2.770173	-0.709770	0.308247
C	3.147047	-2.843464	0.065305
C	2.328290	-3.760167	0.737732
C	4.164973	-3.315005	-0.777895
C	2.515421	-5.134759	0.560968
H	1.546299	-3.404895	1.398745
C	4.342485	-4.689428	-0.953735
H	4.826142	-2.616227	-1.275468
C	3.519740	-5.600858	-0.287694
H	1.873921	-5.836383	1.088458
H	5.132241	-5.046769	-1.610002
H	3.664089	-6.669328	-0.427133
O	3.358924	1.189945	1.060243
C	4.554877	1.595208	0.646216
C	5.071577	2.867977	0.901860
C	5.337449	0.654652	-0.073032
C	6.358350	3.218889	0.446805
C	6.609747	1.005471	-0.522163
C	7.127643	2.290233	-0.265025
Cl	4.080664	3.989905	1.795901
Cl	6.985780	4.816166	0.773525
Cl	8.722918	2.713227	-0.838948
Cl	7.530468	-0.192323	-1.402772

Table S9. XYZ coordinates of [**2**-μ_2-F]$^-$ obtained in the computational mechanistic studies.



Sb	-1.086928	2.080540	-0.262373
Sb	-1.013556	-2.114415	0.260922
Fe	-2.937275	0.306411	2.613021
Fe	-2.923589	-0.406092	-2.614747
Cl	2.261825	3.027516	3.420780
Cl	5.213272	3.449889	2.290407
Cl	5.738524	3.164144	-0.822485
Cl	3.305773	2.457063	-2.757926
Cl	3.386757	-2.342569	2.759834
Cl	5.842906	-2.969677	0.826440
Cl	5.329342	-3.274981	-2.286607
Cl	2.366524	-2.951284	-3.419104
F	-0.472595	-0.008070	-0.001456
O	0.294030	2.384630	1.298751
O	0.735803	2.135250	-1.316421
O	0.808537	-2.107885	1.317032
O	0.377071	-2.370208	-1.299278
C	4.232733	-2.782836	0.172693
C	4.005970	-2.918628	-1.201307
C	2.701069	-2.774913	-1.711506
C	3.154725	-2.502326	1.035427
C	-2.564341	1.827652	1.281737
C	-3.920365	1.376830	1.152167
H	-4.369529	0.975183	0.255518
C	-4.573617	1.540397	2.410797
H	-5.596986	1.267184	2.636152
C	-3.631490	2.103667	3.324025
H	-3.810794	2.324435	4.368989
C	-2.395850	2.281046	2.632698
H	-1.471139	2.658437	3.045761
C	-1.966823	-1.431412	2.063465
C	-3.304511	-1.719537	2.492121
H	-4.071479	-2.206090	1.903419
C	-3.452296	-1.263476	3.836538
H	-4.355825	-1.319741	4.431082
C	-2.206132	-0.698413	4.246533
H	-1.999680	-0.240204	5.205663
C	-1.293289	-0.797462	3.156006
H	-0.272782	-0.441685	3.135579
C	-2.010096	1.361996	-2.066230
C	-3.352434	1.608611	-2.505783
H	-4.138071	2.074358	-1.924899
C	1.628587	-2.496774	-0.862098
C	-3.476556	1.142487	-3.849296
H	-4.376923	1.169406	-4.450659
C	-2.210974	0.613117	-4.247700
H	-1.983867	0.156484	-5.202911
C	-1.309781	0.743841	-3.150918
H	-0.279464	0.418400	-3.120955
C	-2.500048	-1.912160	-1.281878
C	1.859109	-2.356784	0.535314
C	-3.868679	-1.502740	-1.148606
H	-4.326160	-1.112059	-0.251390
C	-4.521216	-1.688932	-2.404410
H	-5.553377	-1.447816	-2.626394
C	-3.565568	-2.224921	-3.319806
H	-3.742236	-2.452881	-4.363683
C	-2.322554	-2.362827	-2.632480
H	-1.388200	-2.712016	-3.048814
C	-1.424804	4.206879	-0.632854
C	-2.271701	4.974190	0.176777
H	-2.761767	4.525210	1.036295
C	-2.491585	6.325714	-0.106488
H	-3.149587	6.910637	0.532658
C	-1.866562	6.922882	-1.202327
H	-2.035837	7.974779	-1.421389
C	-1.018878	6.164900	-2.013286
H	-0.524372	6.624660	-2.865980
C	-0.797584	4.815008	-1.730117
H	-0.128790	4.234626	-2.358440
C	-1.279037	-4.250693	0.631955
C	-0.644441	-4.834624	1.737856
H	-0.004811	-4.229711	2.373537
C	-0.821380	-6.191113	2.020762
H	-0.321622	-6.631903	2.880374
C	-1.631856	-6.979594	1.200883
H	-1.767216	-8.036333	1.420193
C	-2.263692	-6.406511	0.096083
H	-2.892628	-7.015240	-0.550025
C	-2.087818	-5.048539	-0.187114
H	-2.582685	-4.618565	-1.053341
C	1.541089	2.551659	0.862842
C	2.603210	2.864146	1.713309
C	3.903019	3.050854	1.204065
C	4.135005	2.923519	-0.169911
C	3.067539	2.607715	-1.033541
C	1.777090	2.419168	-0.534363

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