Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

A Model for C-F Activation By Electrophilic Phosphonium Cations

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1. Materials and Methods

General Remarks

All preparations and manipulations were carried out under an anhydrous N_2 atmosphere using standard Schlenk and glovebox techniques. All glassware was oven-dried and cooled under vacuum before use. Commercially-available reagents such as 1,8-dibromonaphthalene, isopropylmagnesium bromide (lithium chloride complex) and *n*-butyllithium solutions, iodine, 1,10-phenanthroline, sodium *tert*-butoxide, (trifluoromethyl)trimethylsilane, copper iodide and xenon difluoride were purchased from Sigma Aldrich, Strem or Apollo Scientific and used without further purification unless indicated otherwise. $[Et_3Si(tol)][B(C_6F_5)_4]$[1] was prepared according to literature procedures. 1-Bromo-8-iodonaphthalene was prepared via a modified literature procedure.[2] CH_2Cl_2, *n*-pentane, and toluene were dried using an Innovative Technologies solvent purification system. CD_2Cl_2 (Aldrich) was degassed, distilled over CaH_2, then stored over 4 Å molecular sieves before use. Fluorobenzene was degassed and stored over 4 Å molecular sieves before use.

X-ray Diffraction Studies

A single crystal of **4** was coated with Paratone-N oil, mounted using a polyimide MiTeGen loop and frozen in a cold nitrogen stream (150 K) on the goniometer. Data was collected on a Bruker Apex II CCD diffractometer, using graphite-monochromated MoKα radiation ($\lambda = 0.71073$ Å). Data reduction was performed using the SAINT software package and an absorption correction was applied using SADABS. The structure was solved by direct methods using XS and refined by full-matrix least squares on F^2 using XL as implemented in the SHELXTL suite of programs. All non-hydrogen atoms were refined anisotropically. Carbon-bound hydrogen atoms were placed in calculated positions using an appropriate riding model and coupled isotropic temperature factors.

NMR Spectroscopy

NMR spectra were obtained on a Bruker AvanceIII spectrometer operating at 400.37 MHz ($\nu(^{1}H)$), an Agilent DD2 MHz spectrometer operating at 499.66 MHz ($\nu(^{1}H)$), and an Agilent DD2 spectrometer operating at 599.821 MHz ($\nu(^{1}$H).

Variable temperature 1D ^{19}F and 1D $^{31}P\{^{1}H\}$ NMR spectra were recorded using an Agilent DD2 spectrometer equipped with a 5mm HFX probe (($\nu(^{31}P)$ = 242.81 MHz; ($\nu(^{19}F)$ = 564.33 MHz; ($\nu(^{1}H)$ = 599.821 MHz). ^{19}F NMR spectra were acquired using a standard 1D pulse sequence with 131072 points over a 73529 Hz spectra window, a 30° pulse width, a 10s recycle delay, and 8 transients. 1D $^{31}P\{^{1}H\}$ spectra were acquired using a standard 1D pulse sequence with waltz16 ^{1}H decoupling, as well as 262144 points over a 147059 Hz spectra window, a 30° pulse width, a 0.1s recycle delay, and 128 transients. Samples were allowed to equilibrate for 5 minutes at each temperature prior to NMR acquisition.

2D ^{19}F-^{13}C HSQC and ^{19}F-^{31}P HSQC NMR spectra were also recorded using an Agilent DD2 spectrometer equipped with a 5mm HFX probe (($\nu(^{31}P)$ = 242.81 MHz; ($\nu(^{19}F)$ = 564.33 MHz; $\nu(^{13}C)$ = 150.84 MHz). Both experiments were acquired using the standard vendor-supplied gradient HSQC pulse sequence with decoupling in the indirect dimension. The ^{19}F-^{31}P HSQC experiment was acquired with a 1s recycle delay, 4 transients, 1722 points over a 28409 Hz spectral width in the direct-detect (^{19}F) dimension and 64 increments over a 6070 Hz spectral width in the indirect-detect (^{31}P) dimension. The ^{19}F-^{13}C HSQC experiment was acquired with a 1s recycle delay, 8 transients, 4096 points over a 96153 Hz spectral width in the direct-detect (^{19}F) dimension and 128 increments over a 6070 Hz spectral width in the indirect-detect (^{31}P) dimension. 50% non-uniform sampling was applied in the indirect-detect dimension.

NMR processing was carried out using MestReNova software (v 11.0), Santiago de Compostela, Mestrelab Research S.L., Spain). All 1D NMR spectra were Fourier transformed, phased and then baseline corrected. 2D NMR HSQC spectra were processed using Gaussian apodization functions in F1 and F2, prior to Fourier transformation and phasing. Chemical shifts were either referenced relative to residual solvent peaks ($CDCl_3$ (^{1}H), (^{13}C); CD_2Cl_2 (^{1}H), (^{13}C) or indirectly referenced relative to the spectrometer lock frequency (^{19}F, ^{31}P).

Data for ^{1}H NMR spectroscopy are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, m = multiplet, dm = doublet of multiplets, b = broad), coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift (δ / ppm).

Mass Spectrometry

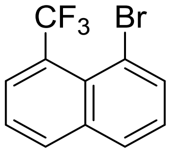
High-resolution mass spectra (HRMS) were obtained on a micro mass 70S-250 spectrometer (EI), an ABI/Sciex QStar Mass Spectrometer (DART), or on a JOEL AccuTOF-DART (DART). Mass spectrometry experiments were run for isolated products and reaction mixtures, however in some cases the high fragmentation of compounds or volatility did not allow for mass peak identification.

Computational Details

Electronic structure calculations were performed using density functional theory (DFT) as implemented in the Gaussian 09 program (revision E.01).[3] The geometry of the cation of compound **4** was optimized at the B3LYP/def2-SVP level of theory using the crystallographic coordinates as the input geometry. The stationary nature of the converged-upon geometry was confirmed by carrying out a frequency calculation and ensuring the absence of imaginary frequencies. NBO calculations were performed with NBO version 6.[4] Atoms in molecules analyses[5-7] were performed for the cation **4** using MultiWFN.

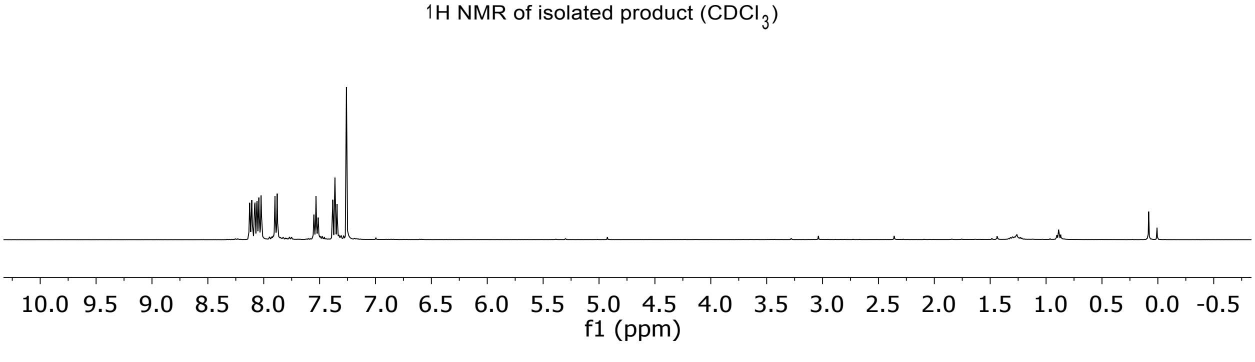
2. Syntheses and Spectroscopic Data of Compounds 1-4

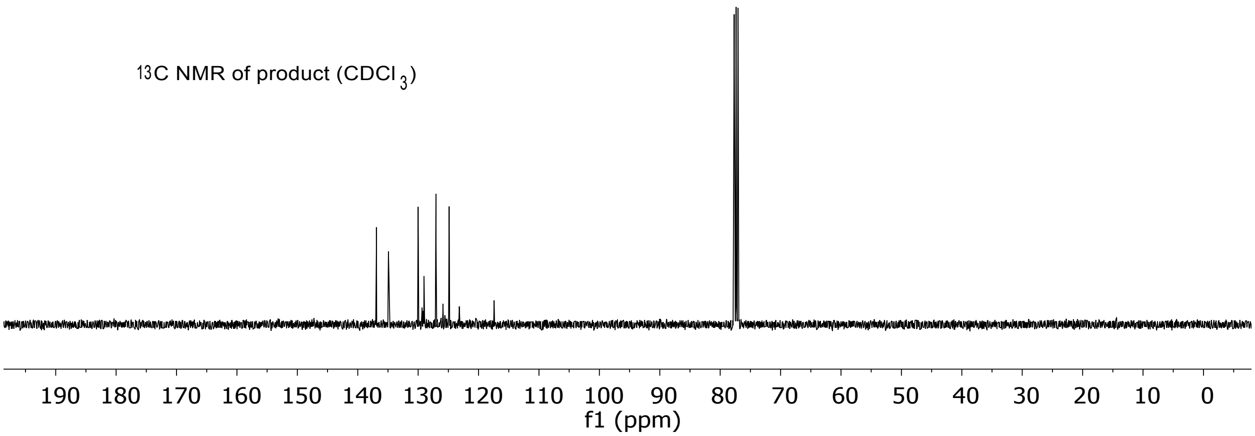
2.1 Synthesis of 8-Trifluoromethyl-1-bromonaphthalene 1[8,9]

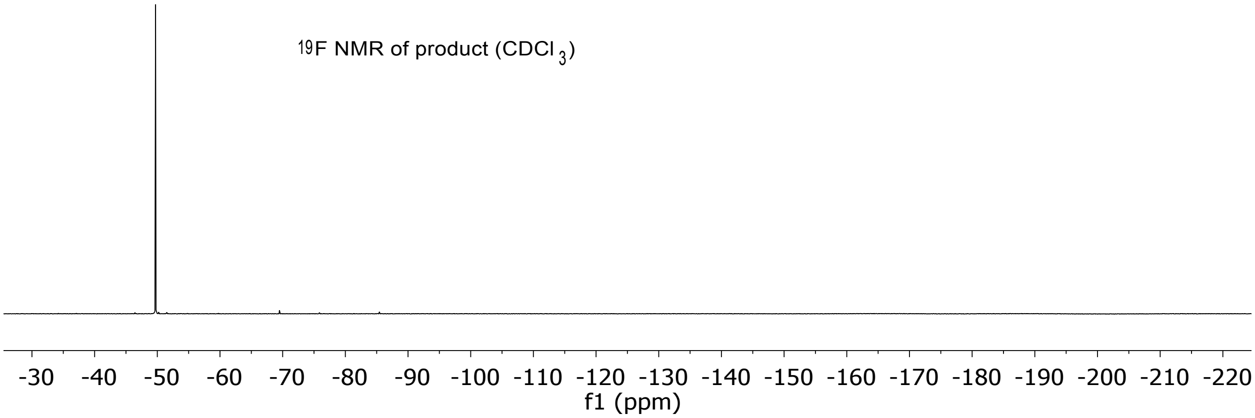


To an oven-dried 100 mL Schlenk flask was added copper iodide (198 mg, 2.00 mmol, 2.00 equiv). Air in the flask was then evacuated and the flask was re-filled with nitrogen. Under positive pressure of nitrogen, KO*t*Bu (224 mg, 2.00 mmol, 2.00 equiv) and 1,10-

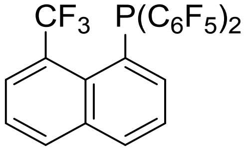
phenanthroline (360 mg, 2.00 mmol, 2.00 equiv) were then added, along with 4.0 mL DMF. The Schlenk flask was sealed under nitrogen and the dark red mixture was stirred for 30 min. $TMSCF_3$ (0.296 mL, 2.00 mmol, 2.00 equiv) was then added via syringe and the mixture was stirred for a further 60 min. The stopper was then removed and, under a positive pressure of nitrogen, 1-bromo-8-iodonaphthalene was added quickly via powder funnel. The Schlenk flask was then sealed and the mixture was stirred under nitrogen for 18 h at 50 °C. The mixture was then cooled, diluted with 15 mL Et_2O, and filtered through Celite. The Celite was washed with a further 5 mL Et_2O and the combined organic layers were washed sequentially with 10 mL 1 M HCl, 10 mL aqueous $NaHCO_3$ solution, and 10 mL brine, and dried over Na_2SO_4. The yellow solution was then concentrated and placed in a refrigerator at 0 °C overnight, affording brown-tinged yellow, x-ray-quality crystals of **5-8** in 68% yield. **^{1}H NMR ($CDCl_3$ [ppm]):** $\delta = 7.36$ (t, $^3J_{HH} = 7.8$ Hz, 1H, Ar), 7.53 (t, $^3J_{HH} = 7.8$ Hz, 1H, Ar), 7.88 (dd, $^3J_{HH} = 8.0$ Hz, $^4J_{HH} = 1.2$ Hz, 1H, Ar), 8.03 (dd, $^3J_{HH} = 8.3$ Hz, $^4J_{HH} = 1.3$ Hz, 1H, Ar), 8.07 (dd, $^3J_{HH} = 7.5$ Hz, $^4J_{HH} = 1.3$ Hz 1H, Ar), 8.12 (dd, $^3J_{HH} = 7.4$ Hz, $^4J_{HH} = 1.2$ Hz, 1H, Ar), **^{13}C{^{1}H} NMR ($CDCl_3$, [ppm])**: 117.4 (s, C*Ar*), 124.9 (s, C*Ar*), 127.0 (s, C*Ar*), 129.0 (q, $J_{FC} = 8.0$ Hz, C*Ar*), 129.4 (s, C*Ar*), 130.0 (s, C*Ar*), 134.9 (q, $J_{FC} = 1.3$ Hz, C*Ar*), 136.9 (s, C*Ar*), 137.1 (s, C*Ar*). Resonances for two quaternary carbon atoms were not observed. **^{19}F{^{1}H} NMR ($CDCl_3$, [ppm]):** $\delta = -49.7$ (s, CF_3)







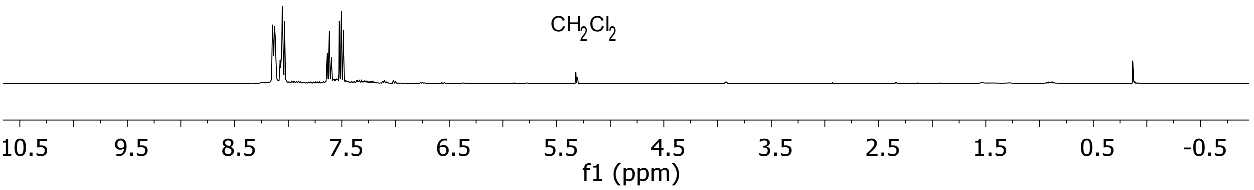
2.2 Synthesis of (8-Trifluoromethylnaphthyl)bis(pentafluorophenyl)fluorophosphine 2



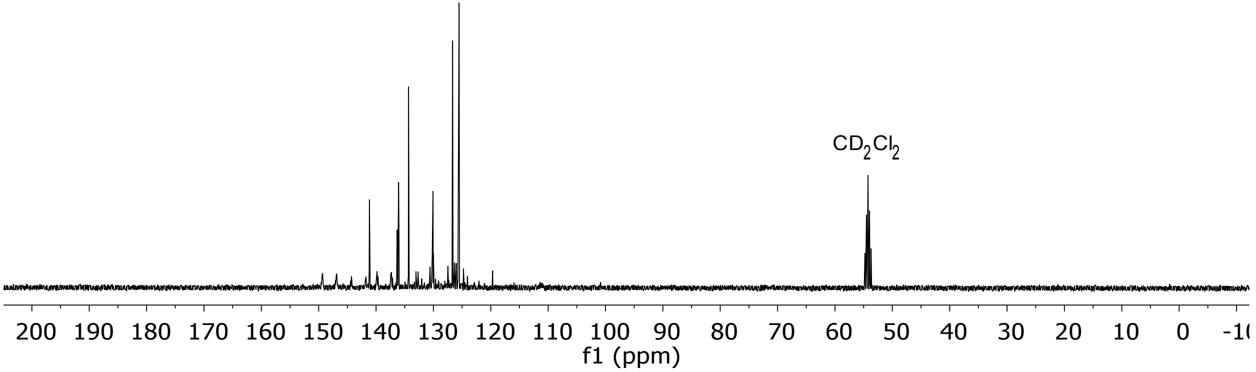
A solution of **5-8** (68.8 mg, 0.25 mmol) in toluene was cooled to –35 °C. 0.10 mL (0.25 mmol) of a 2.5 M solution of *n*BuLi in hexanes was added dropwise. Allowing the mixture to warm to room temperature over 2 h resulted in a brown suspension. The brown suspension was cooled to –35 °C and a cooled solution of $(C_6F_5)_2PBr$ (111.0 mg, 0.25 mmol) in 0.5 mL toluene was added dropwise, resulting in change of the colour of the suspension to dull red. This suspension was allowed to warm to room temperature over the course of 20 h. Volatiles were then removed *in vacuo* and the product extracted with 2 mL pentane, which was loaded onto a small silica column. Washing the column with pentane until the yellow colour had reached the bottom of the silica resulted in removal of impurities, and the product was eluted from the column with DCM. This procedure was repeated a second time, affording **5-10** as a sticky white solid in

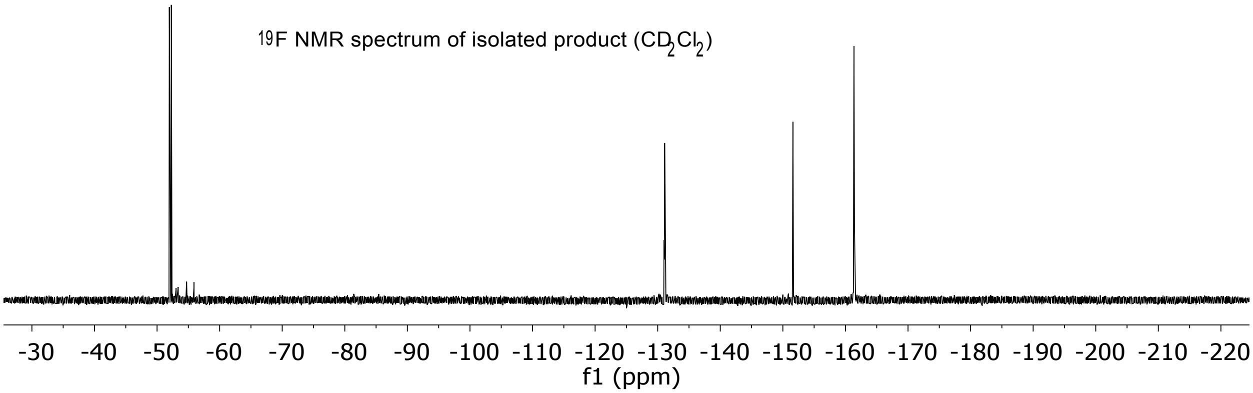
54% yield. **^{1}H NMR (CD$_2$Cl$_2$, [ppm]):** 7.51 (dd, 1H, H*Ar*, $^3J_{\mathrm{HH}}$ = 8.3 Hz, $^3J_{\mathrm{HH}}$ = 7.8 Hz, Ar), 7.62 (dd, 1H, H*Ar*, $^3J_{\mathrm{HH}}$ = 8.3 Hz), 8.03 (2H, m, H*Ar*), 8.13 (2H, dd, $^3J_{\mathrm{HH}}$ = 7.7 Hz, $^3J_{\mathrm{HH}}$ = 3.4 Hz). **^{13}C{^{1}H} NMR (CD$_2$Cl$_2$, [ppm]):** δ = 119.7 (m, C, *C*F$_3$), 126.1 (d, 1C, CAr, $^1J_{\mathrm{PC}}$ = 114 Hz), 130.1 (q, 1C, CAr, $^4J_{\mathrm{FC}}$ = 7.3 Hz), 132.9 (d, $^2J_{\mathrm{PC}}$ = 37 Hz, CAr) 134.3 (s, 1C, CAr), 136.1 (m, 1C, CAr), 136.3 (d, 1C, CAr, $^4J_{\mathrm{PC}}$ = 8.4 Hz), 141.2 (q, 1C, Car, $^1J_{\mathrm{FC}}$ = 2.0 Hz), 138.7 (d of m, 2C, *m-C$_6$F$_5$*, $^1J_{\mathrm{FC}}$ = 255 Hz), 143.0 (d of m, 1C, C, *p-C$_6$F$_5$*, $^1J_{\mathrm{FC}}$ = 255 Hz), 148.1 (d of m, 2C, *o-C$_6$F$_5$* $^1J_{\mathrm{FC}}$ = 248 Hz). Resonances for *ipso*-carbon atoms on phenyl moieties were not observed. **^{19}F{^{1}H} NMR (CD$_2$Cl$_2$, [ppm]):** –52.1 (d, 3F, C*F$_3$*, J_{PF} = 120 Hz),), –131.1 (t, 4F, *o-C$_6$F$_5$*, $^3J_{\mathrm{FF}}$ = 29 Hz), –151.5 (t, 2F, *p-C$_6$F$_5$*, $^3J_{\mathrm{FF}}$ = 21 Hz), –161.4 (td, 4F, *m-C$_6$F$_5$*, $^3J_{\mathrm{FF}}$ = 29 Hz, $^3J_{\mathrm{FF}}$ = 21 Hz). **^{31}P{1H} NMR (CD$_2$Cl$_2$, [ppm]):** –34.7 (m) Elemental Analysis for $C_{22}H_{19}F_2P$: calcd.: C 49.3, H 1.1, found: C 50.2, H 1.2; **DART MS:** m/z 561.00821 (calcd. for MH$^+$: 561.00778)

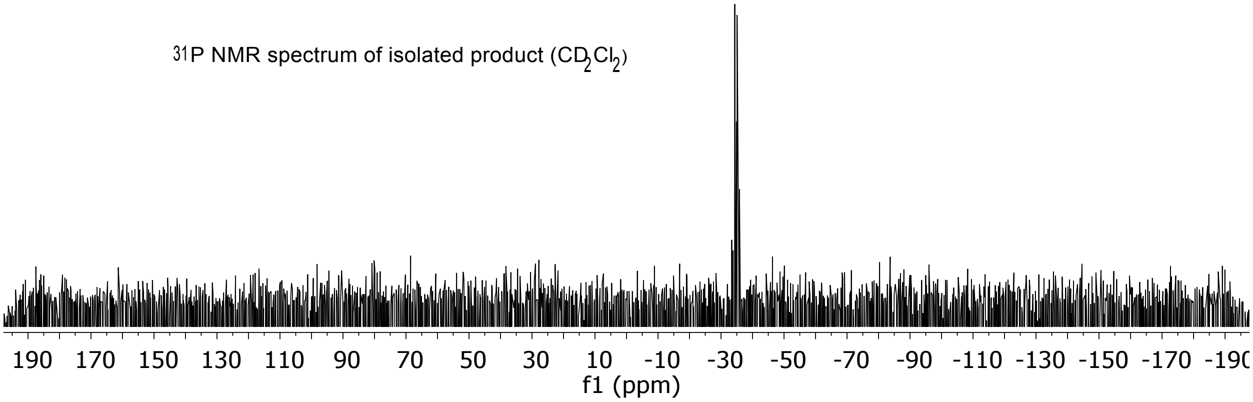
^{1}H NMR spectrum of isolated product (CD$_2$Cl$_2$)



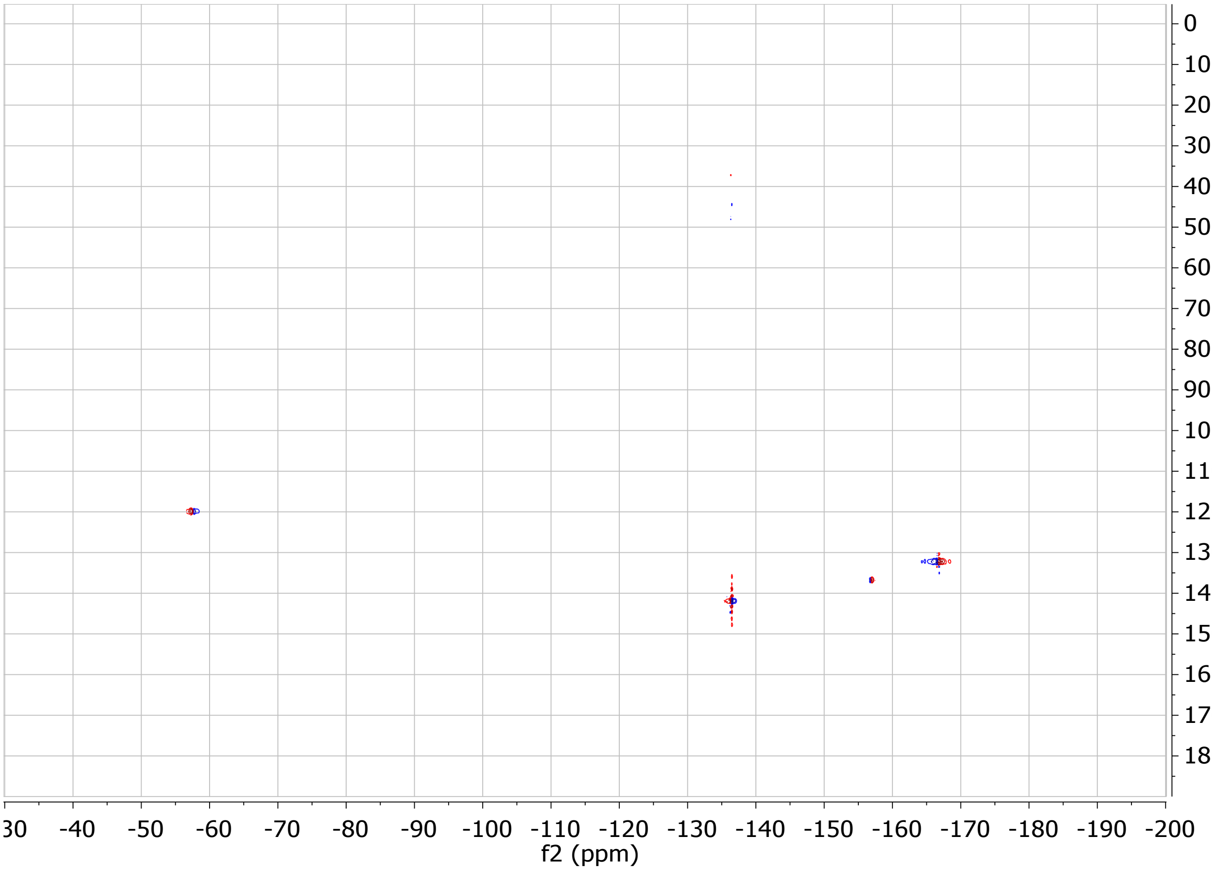
^{13}C NMR spectrum of isolated product (CD$_2$Cl$_2$)



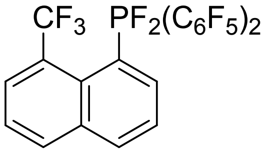

19F NMR spectrum of isolated product (CD2Cl2)
-30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)


31P NMR spectrum of isolated product (CD2Cl2)
190 170 150 130 110 90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190
f1 (ppm)

^{19}F-^{13}C- HSQC spectrum of **2** showing 1-bond F-C correlations of the CF_3 and C_6F_5 moieties

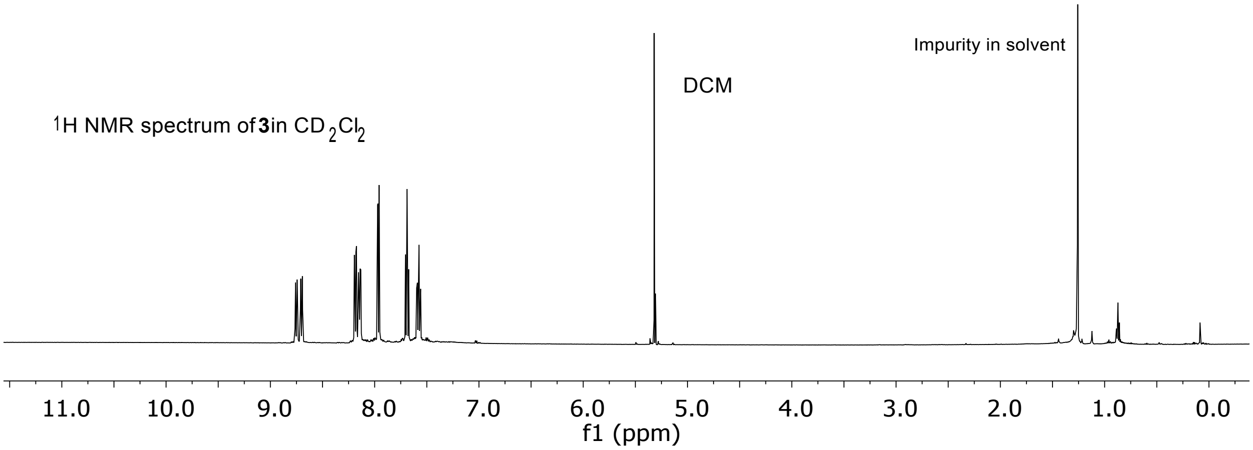


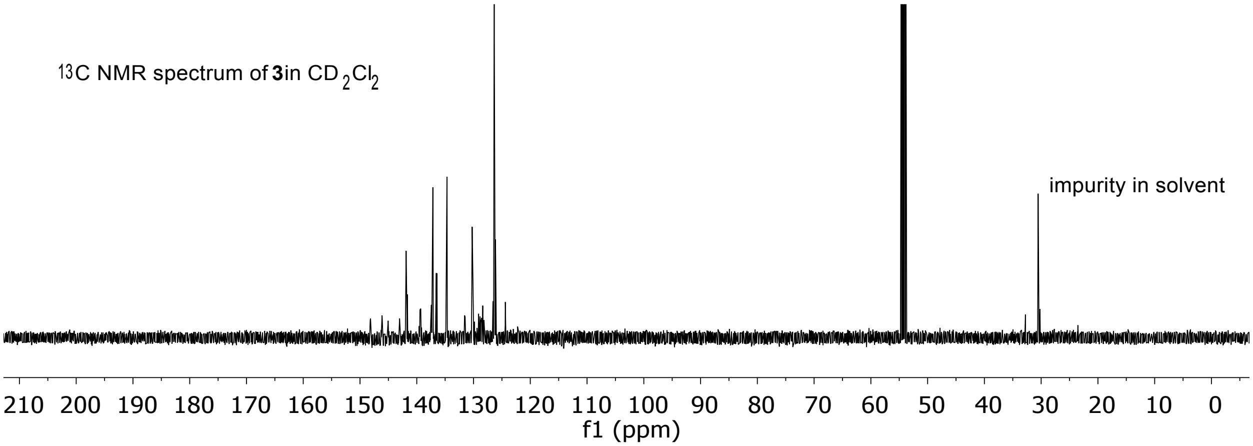
2.3 Synthesis of (8-Trifluoromethylnaphthyl)bis(pentafluorophenyl)difluorophosphorane 3

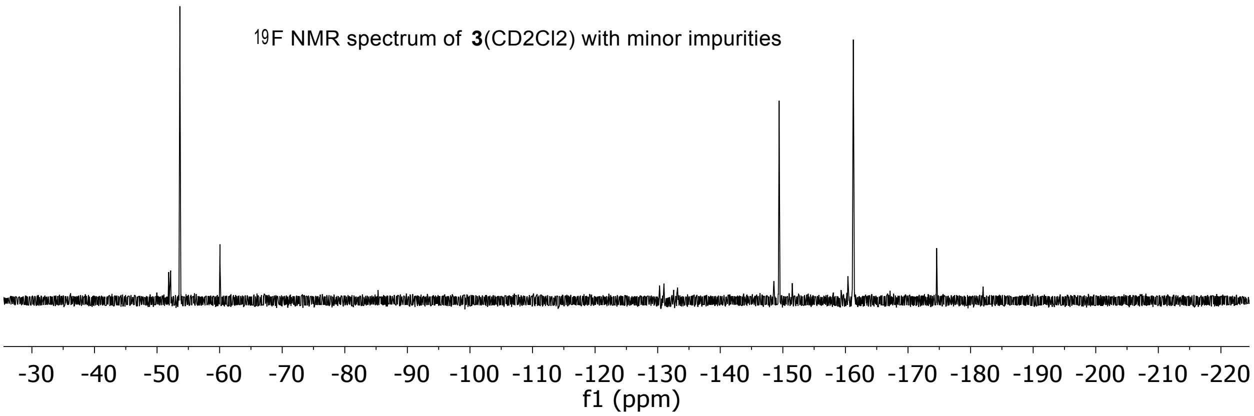


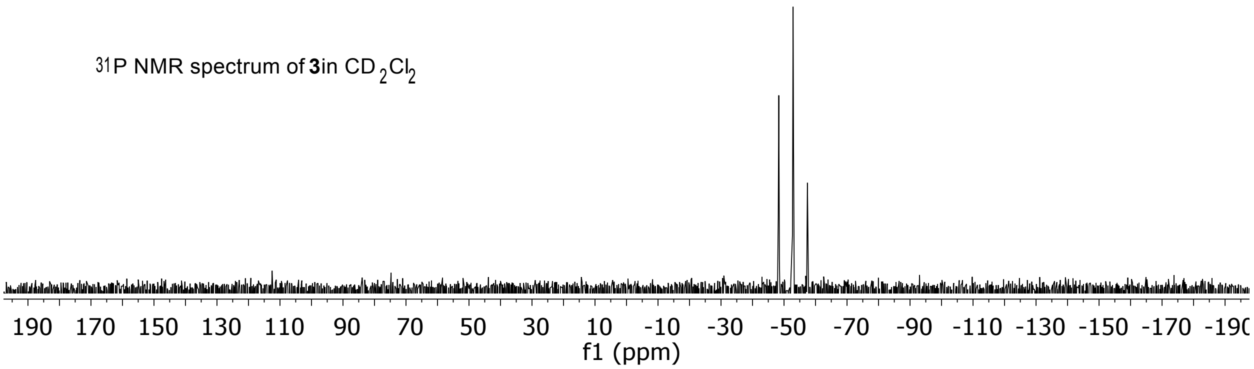
To a solution of **2** (54 mg, 0.096 mmol) in DCM was added a DCM solution containing 16 mg (1.0 equiv., 0.096 mmol) XeF_2. The solution was allowed to stir for 2 h. Volatiles were then removed *in vacuo* and the resultant solid washed with 1 mL *n*-pentane, affording **3** as a white solid in 86% yield. **^{1}H NMR (CD_2Cl_2, [ppm]):** 7.58 (td, 1H, H*Ar*, $^3J_{HH}$ = 7.8 Hz, $^4J_{HH}$ = 3.6 Hz), 7.69 (t, 1H, H*Ar*, $^3J_{HH}$ = 7.7 Hz), 7.96 (dd, 1H, H*Ar*, $^3J_{HH}$ = 7.4 Hz, $^4J_{HH}$ = 1.4 Hz), 8.14 (dd, 1H, H*Ar*, $^3J_{HH}$ = 8.1 Hz, $^4J_{FH}$ = 3.3 Hz), 8.18 (1H, ddd, H*Ar*, $^3J_{HH}$ = 8.1 Hz, $^4J_{PH}$ = 2.9 Hz, $^4J_{HH}$ = 1.2 Hz), 8.73 (ddd, 1H, H*Ar*, $^3J_{PH}$ = 25 Hz, $^3J_{HH}$ = 7.6 Hz, $^4J_{HH}$ = 1.2 Hz). **^{13}C{^{1}H} NMR**

(CD$_2$Cl$_2$, [ppm]): 124.4 (s, C*Ar*), 126.2 (d, C*Ar*, $^3J_{PC}$ = 21.7 Hz), 126.3 (s, C*Ar*), 128.4 (t, CAr), 129.0 (d, $^3J_{PC}$ = 26.8 Hz), 130.3 (q, CAr, $^4J_{FC}$ = 5.1 Hz), 131.5 (d, $^4J_{PC}$ = 12.6 Hz, C*Ar*), 134.7 (s, C*Ar*), 136.5 (d, C*Ar*, $^4J_{PC}$ = 9.9 Hz), 137.2 (d, C*Ar*, $^5J_{PC}$ = 5.2 Hz), 141.8 (q, C*Ar*, $^3J_{FC}$ = 13.7 Hz**)**, 138.4 (d of m, *m*-C_6F_5, $^1J_{FC}$ = 252 Hz), 144.0 (d of m, *p*-C_6F_5, $^1J_{FC}$ = 259 Hz), 147.1 (d of m, *o*-C_6F_5, $^1J_{FC}$ = 248 Hz). Resonances for *ipso*-carbon atoms on C$_6$F$_5$ rings were not observed. **^{19}F{^{1}H} NMR (CD$_2$Cl$_2$, [ppm]):** –53.6 (s, C*F$_3$*), –133.1 (4F, m(br)), –149.9 (2F, t, *p*-C_6F_5, $^3J_{FF}$ = 21 Hz), –161.3 (4F, m, *m*-C_6F_5). **^{31}P{1H} NMR (CD$_2$Cl$_2$, [ppm]):** –53.0 (t, $^1J_{PF}$ = 736 Hz)

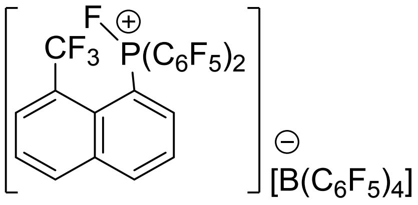






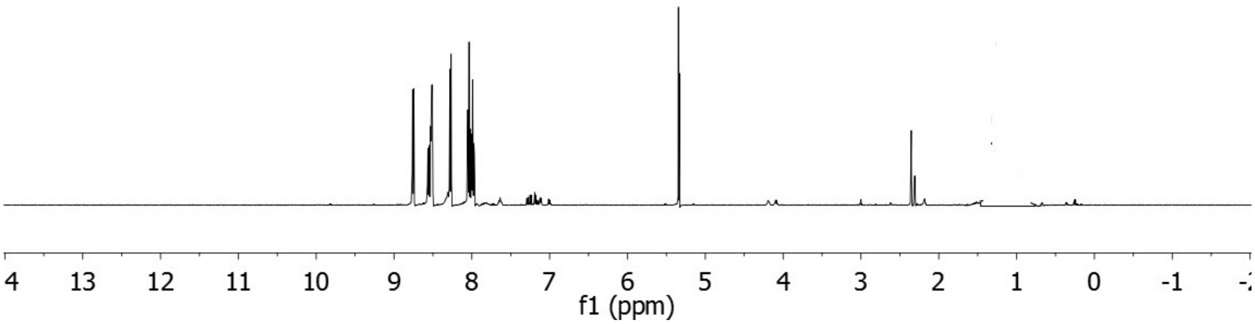


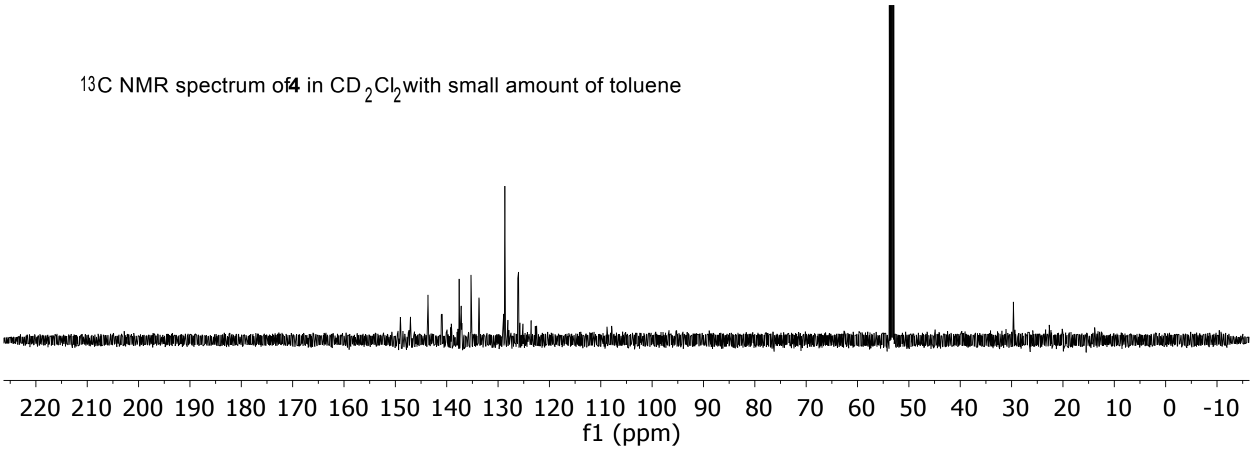
2.4 Synthesis of (8-Trifluoromethylnaphthyl)bis(pentafluorophenyl)fluorophosphonium salt 4

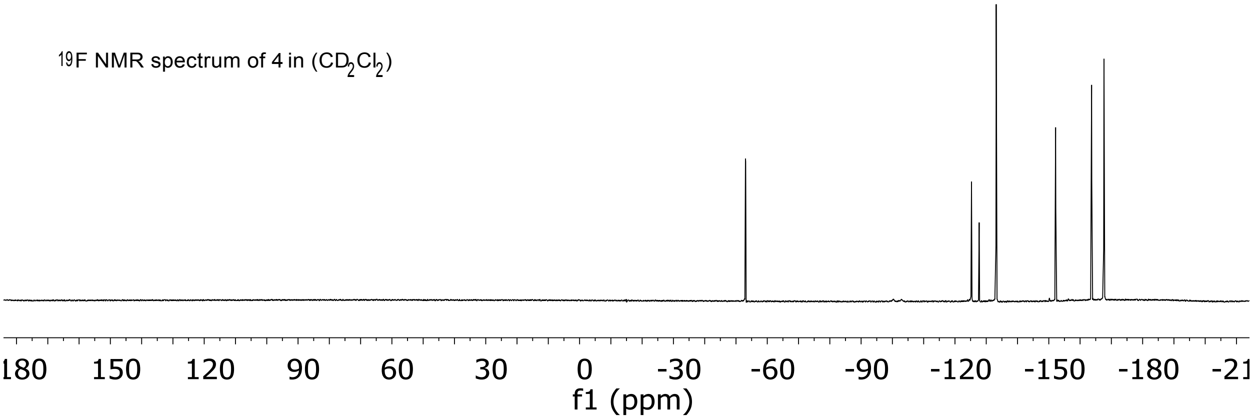


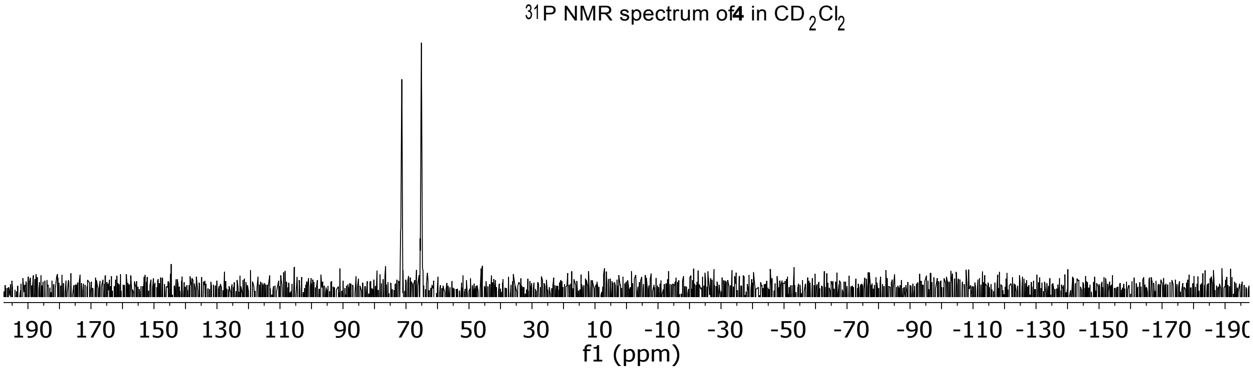
To a vial containing **4** (54 mg, 0.90 mmol) was added 76 mg $[Et_3Si(tol)][B(C_6F_5)_4]$ (0.86 mmol, 0.95 equiv.) in several portions, with shaking after each addition. Immediately a dark, oily precipitate formed on the bottom of the vial. The vial was left to stand for 4 h then the supernatant was decanted from the oily precipitate and the precipitate was washed with toluene (2 x 0.5 mL) and n-pentane (2 x 0.5 mL) and dried *in vacuo* yielding 70 mg of **4** (65% yield). X-ray quality crystals were obtained by slow diffusion of *n*-pentane into a saturated solution of **4** in DCM cooled to -35 °C. **^{1}H NMR (CD_2Cl_2, [ppm]):** 7.96 (1H, td, $^3J_{HH}$ = 8.0 Hz, $^4J_{HH}$ = 3.1 Hz, H*Ar*), 8.01 (1H, ddd, $^3J_{HH}$ = 8.3 Hz, $^3J_{HH}$ = 7.5 Hz, $^4J_{HH}$ = 1.0 Hz), 8.25 (1H, dd, $^3J_{HH}$ = 7.6 Hz, $^4J_{HH}$ = 1.3 Hz, H*Ar*), 8.52 (2H, m, H*Ar*), 8.73 (1H, d, $^3J_{HH}$ = 8.3 Hz). **$^{13}C\{^1H\}$ NMR (CD_2Cl_2, [ppm]):** δ = 127.7 (d, J_{PC} = 18 Hz, C*Ar*), 129.5 (s, C*Ar*), 134.6 (q, $^4J_{FC}$ = 5.4 Hz, C*Ar*), 136.2 (d, J_{PC} = 13.5 Hz, CAr) 138.0 (s, C*Ar*), 138.4 (m, C*Ar*), 138.7 (dm, *m*-$C_6F_{5,}$), 139.6 (dm, $^1J_{FC}$ = 262 Hz, C_6F_5), 141.8 (m, C*Ar*), 144.5 (d, CAr, J_{PC} = 3.6 Hz), 148.6 (dm, C_6F_5), 148.9 (dm, $^1J_{FC}$ = 242 Hz, C_6F_5), 150.2 (dm, C_6F_5 $^1J_{FC}$ = 270 Hz). Resonances for *ipso*-carbon atoms on C_6F_5, phenyl moieties, CF_3 were not observed. **$^{19}F\{^1H\}$ NMR (CD_2Cl_2, [ppm]):** –53.1 (3F, d, C$F_{3,}$ J_{PF} = 27 Hz), –125.3 (4F, m, *o*-P(C_6F_5)$_2$), –127.7 (2F, m, *p*-P(C_6F_5)$_2$), –133.3 (8F, m, *o*-B(C_6F_5)$_4$, – 152.2 (4F, tm, $^3J_{FF}$ = 19 Hz, *m*-P(C_6F_5)$_2$), –163.7 (4F, td, $^3J_{FF}$ = 21 Hz *p*-B($C_6F_{5,}$)$_4$), –167.6 (8F, m, *m*-B($C_6F_{5,}$)$_4$). Resonance for P-F ^{19}F nucleus was observed at –100.4 ppm at –80 °C but not observed at room temperature. **$^{31}P\{1H\}$ NMR (CD_2Cl_2, [ppm]):** 70.3 (d, $^1J_{PF}$= 1010 Hz).

^1H NMR of **4** in CD_2Cl_2 with small amount of toluene

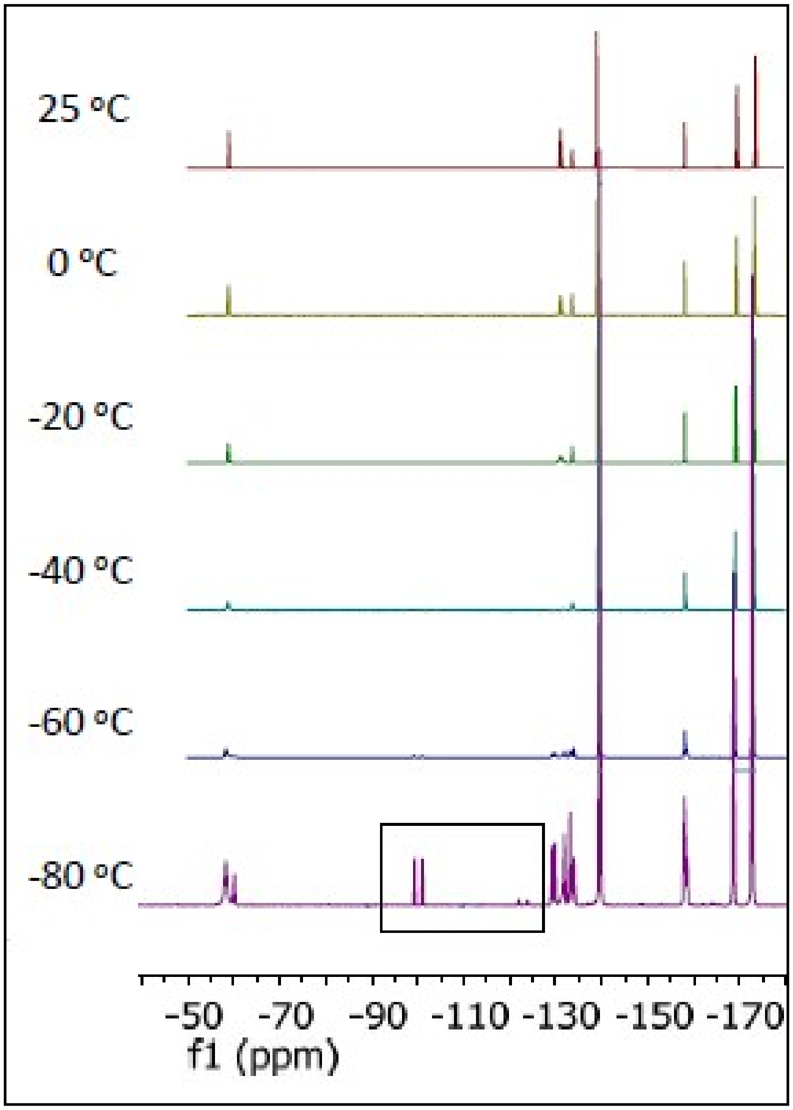



^{13}C NMR spectrum of**4** in $CD_2Cl_2$with small amount of toluene

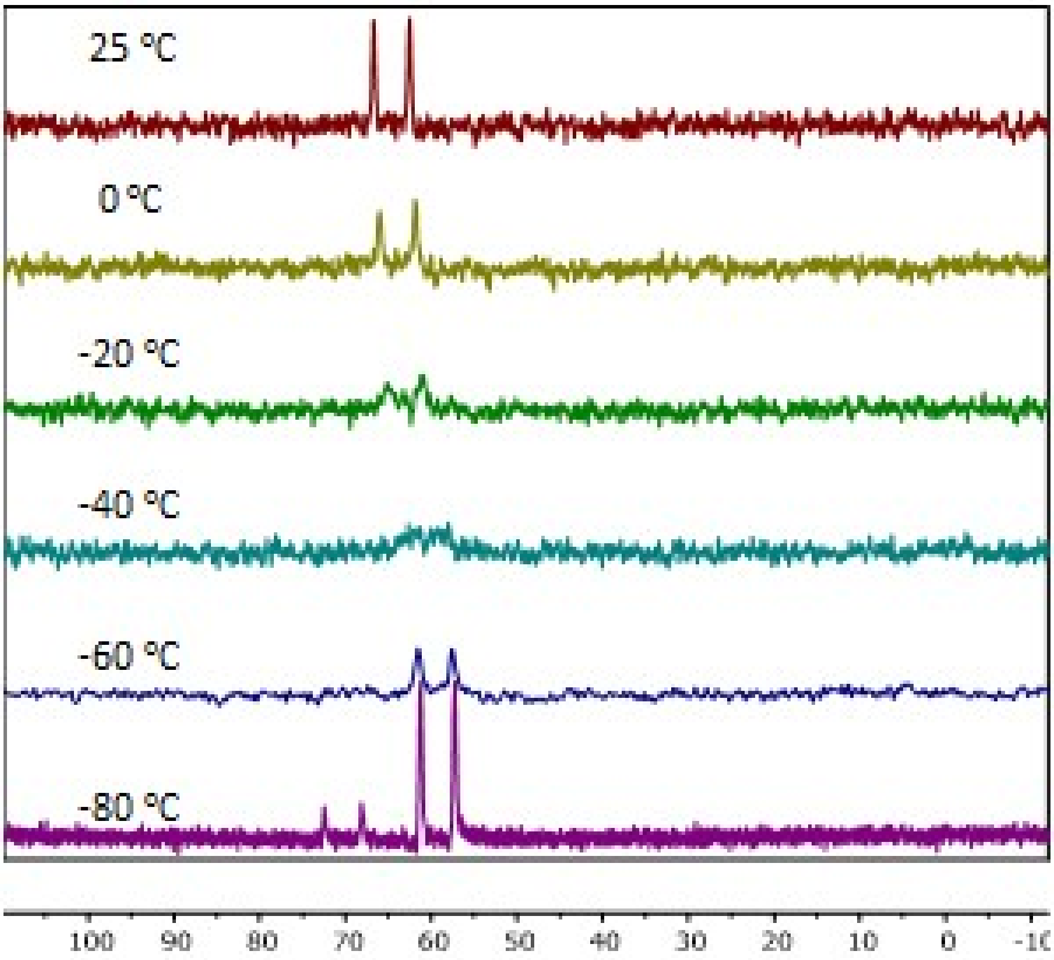

^{19}F NMR spectrum of 4 in (CD_2Cl_2)
180
150
120
90
60
30
0
-30
-60
-90
-120
-150
-180
-21
f1 (ppm)


^{31}P NMR spectrum of **4** in CD_2Cl_2
190
170
150
130
110
90
70
50
30
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-19
f1 (ppm)

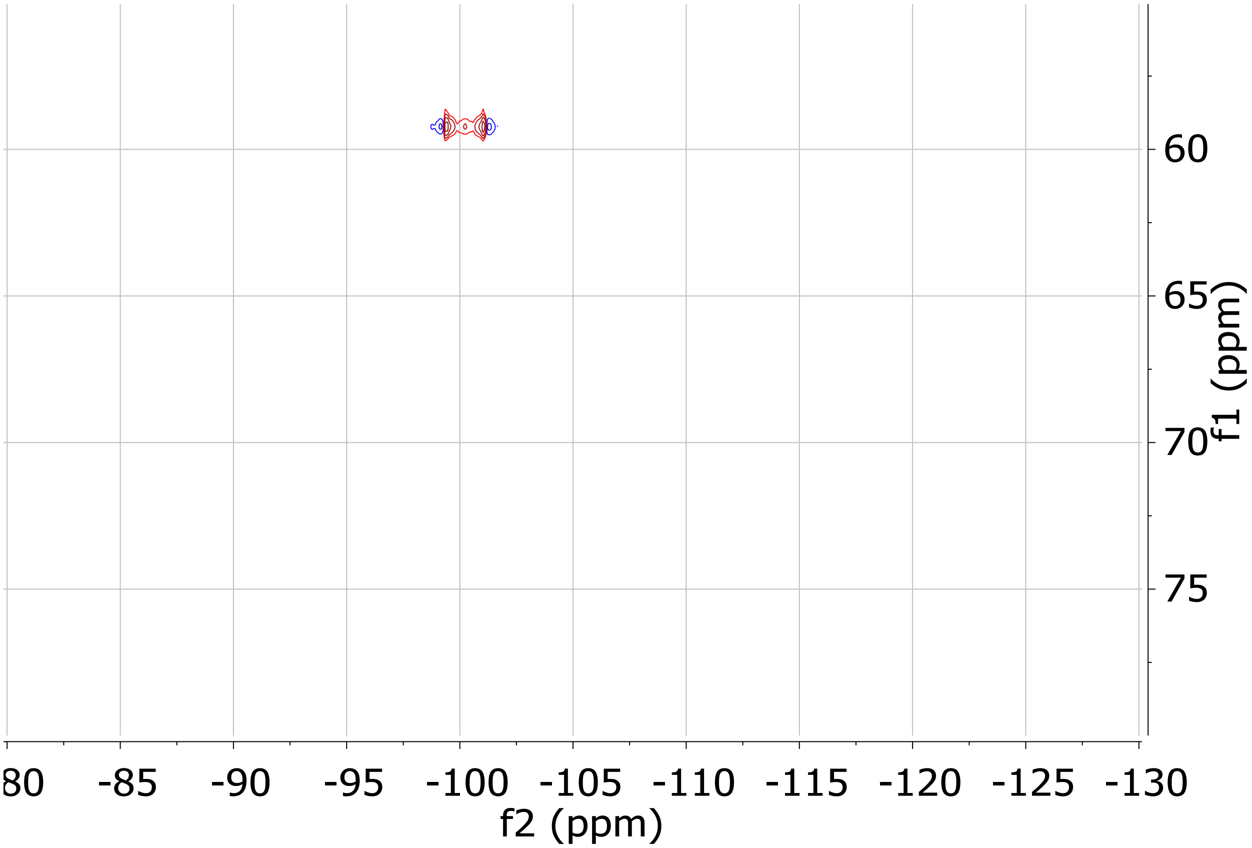
Variable-temperature ^{19}F NMR spectra of **4** in CD_2Cl_2.



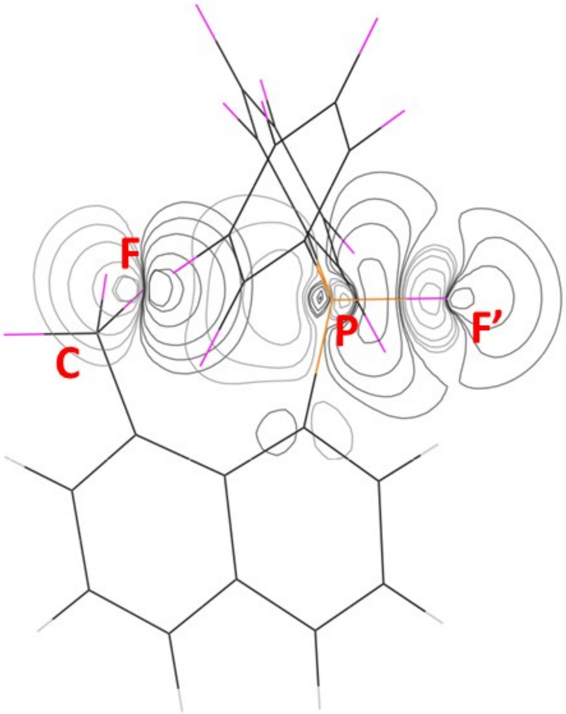
Variable-temperature ^{31}P NMR spectra of **4** in CD_2Cl_2



^{19}F-^{31}P HSQC spectrum of **4** obtained at – 80°C showing a correlation between the ^{31}P NMR resonance at 59.3 ppm (y-axis) and ^{19}F NMR resonance at at – 100.4 ppm (x-axis) for the major species.



Contour plot of the NBO donor-acceptor interaction in compound **4**. The contour map is plotted in the F-P-F' plane and the molecule is depicted as lines with F pink, C black, P orange, and H white.



3. Cartesian Coordinates (Å) for the Optimized Structure of the cation of 4 (Table S1)

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 Center     Atomic      Atomic              Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
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      1         15           0        9.711915   11.636109    2.622594
      2          9           0        9.029671   12.303241    5.024836
      3          9           0        6.875014   12.678469    3.296976
      4          9           0       11.083099   13.806139    4.312327
      5          9           0       10.038179   11.288247    1.114996
      6          9           0        9.376350    8.767796    2.486537
      7          9           0        7.866632   10.621975    5.720963
      8          9           0        8.869759   11.887833    7.118686
      9          9           0        8.001330   13.139234    0.814438
     10          9           0       10.852351   16.460915    4.000622
     11          9           0        4.782567    8.516306    3.303978
     12          9           0        7.791858   15.825311    0.498895
     13          9           0        4.653840   11.198837    3.546525
     14          9           0        7.132474    7.285382    2.788242
     15          9           0        9.228308   17.462928    2.097494
     16          6           0       11.187873   10.398154    4.820344
     17          6           0        8.993702   11.304538    5.941459
     18          6           0        8.225955    9.361795    2.746133
     19          6           0        8.184385   10.756780    2.871734
     20          6           0        5.800715   10.617893    3.288315
     21          6           0       10.218970   10.427738    5.876813
     22          6           0        6.955646   11.373261    3.137307
     23          6           0       10.168738   15.651054    3.228408
     24          6           0        9.553782   13.407593    2.552172
     25          6           0        7.082410    8.590658    2.903513
     26          6           0        8.585907   15.323533    1.412674
     27          6           0       11.131995   11.011753    3.509752
     28          6           0        8.710574   13.952337    1.574158
     29          6           0       10.393056    9.677668    7.025179
     30          1           0        9.636684    9.739328    7.809844
     31          6           0       10.281011   14.272767    3.379561
     32          6           0       12.392727    9.668595    5.102713
     33          6           0       12.244609   11.026879    2.677424
     34          1           0       12.192145   11.493359    1.692609
     35          6           0        9.327220   16.170553    2.242829
     36          6           0        5.867178    9.228009    3.165083
     37          6           0       11.531426    8.881321    7.233911
     38          1           0       11.630237    8.295422    8.147228
     39          6           0       12.528968    8.911506    6.296061
     40          1           0       13.456624    8.358394    6.452042
     41          6           0       13.497501    9.697456    4.208590
     42          1           0       14.396652    9.143968    4.485298
     43          6           0       13.452011   10.403377    3.037240
     44          1           0       14.306661   10.445066    2.363061
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4. Crystallographic data and details of the structure refinement of compound **4** (Table S2)

	$4\cdot CH_2Cl_2$
formula	$C_{48}H_8PF_{34}Cl_2B$
M_r [g mol^{-1}]	1343.22
colour, habit	yellow, needle
crystal system	Triclinic
space group	$P\bar{1}$
a [Å]	12.0867(19)
b [Å]	14.713(3)
c [Å]	27.639(5)
α [°]	90.302(7)
β [°]	97.601(7)
γ [°]	99.450(8)
V [Å^3]	4803.8(14)
Z	4
crystal size [mm^3]	0.9x0.2x0.2
ρ_c [g cm^{-3}]	1.857
F(000)	2624
θ min [°]	0.744
θ max [°]	24.407
reflection area	$-14 \leq h \leq 13$ $-17 \leq h \leq 17$ $-32 \leq h \leq 32$
μ [mm^{-1}]	0.340
absorption correction	SADABS
reflections collected	37892
reflections unique	15465
R_{int}	0.0946
reflections obs. [$F > 2\sigma(F)$]	7165
residual density [e Å^{-3}]	3.362, –0.876
parameters	1569
GOF	1.036
R_1 [$I > 2\sigma(I)$]	0.0976
wR_2 (all data)	0.3236

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