Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information for

Homolytic Cleavage of Peroxide Bonds via a Single Electron Transfer of Frustrated Lewis Pair

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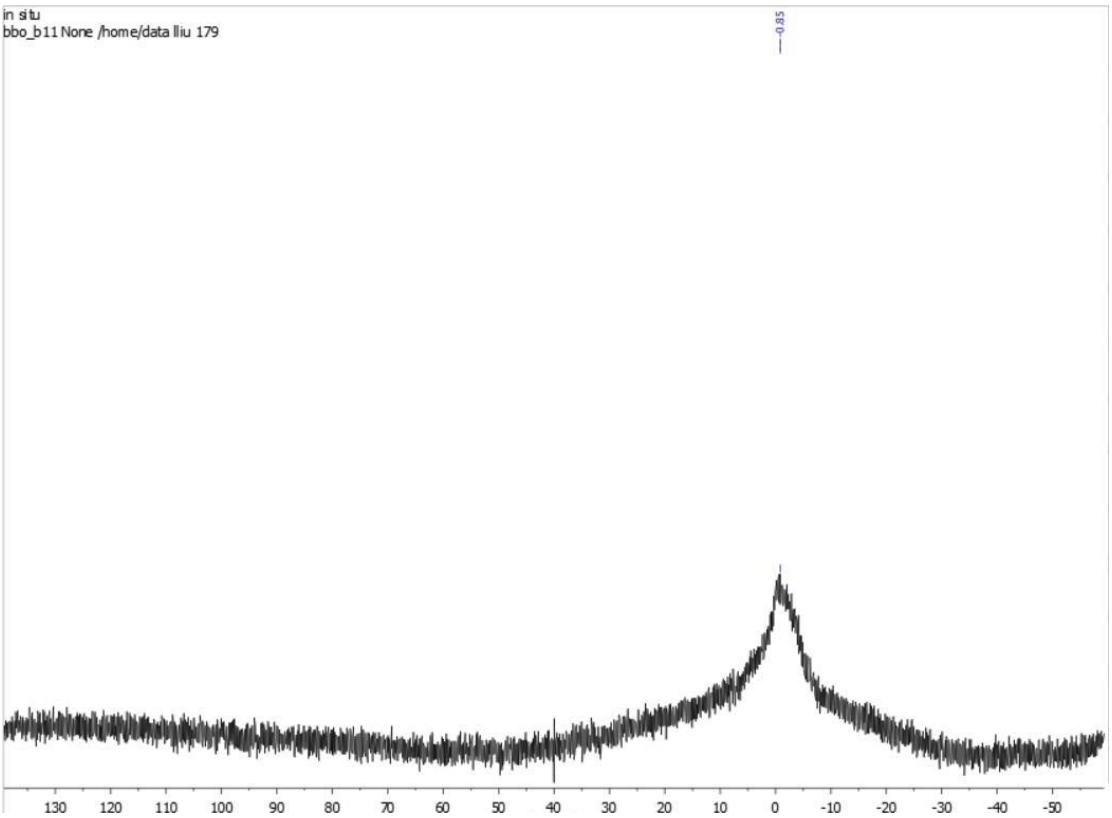
Contents:

General:

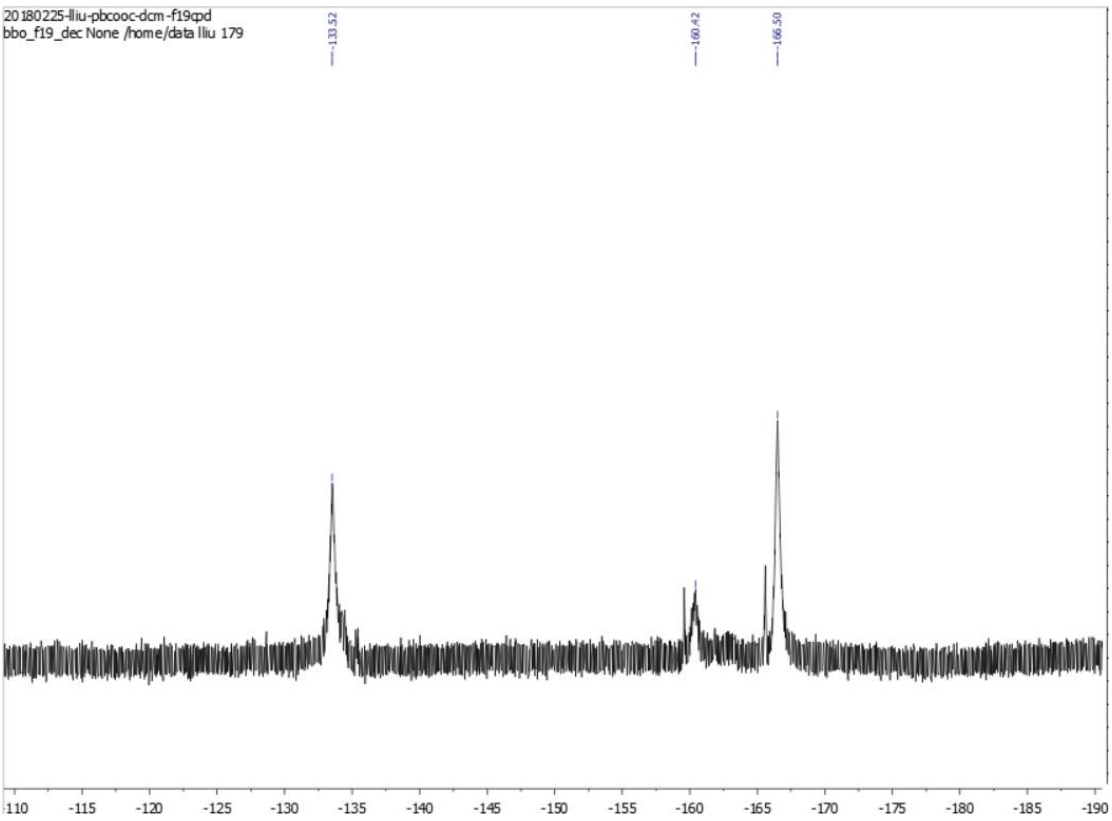
All manipulations were performed under an atmosphere of dry, oxygen-free N_2 by means of standard glovebox techniques (MBraun LABmaster SP drybox and Innovation Technology glovebox both equipped with a −35 °C freezer). Pentane, and dichloromethane (DCM) were collected from a Grubbs-type column system manufactured by Innovative Technology. These solvents were dried over 4 Å molecular sieves. Molecular sieves, type 4 Å (pellets, 3.2 mm diameter) purchased from Sigma-Aldrich were activated prior to usage by iteratively heating with 1050 W Haier microwave for 5 min and cooling under vacuo. The process was repeated until no further moisture was released upon heating. Chloroform-d ($CDCl_3$), purchased from Cambridge Isotope Laboratories, was degassed and stored over 4 Å molecular sieves in the glovebox for at least 8 h prior to use. Ph_3SnH, $(PhCOO)_2$ and Mes_3P were purchased and used directly. $B(C_6F_5)_3$ was purified from sublimation at 100 °C followed by stirring with chlorodimethylsilane at room temperature for 2 h, and dried under vacuo. $(p\text{-}BrC_6H_4COO)_2$ and $(p\text{-}MeC_6H_4COO)_2$ were synthesized according to the literature procedure.[S1] Spectra were recorded on a Bruker Avance III 400 MHz spectrometer and spectra were referenced to residual solvents of $CDCl_3$ (^1H = 7.26 ppm; ^{13}C = 77.0 ppm). Chemical shifts (δ) are reported in ppm and the absolute values of the coupling constants (*J*) are in Hz.

Experimental Section:

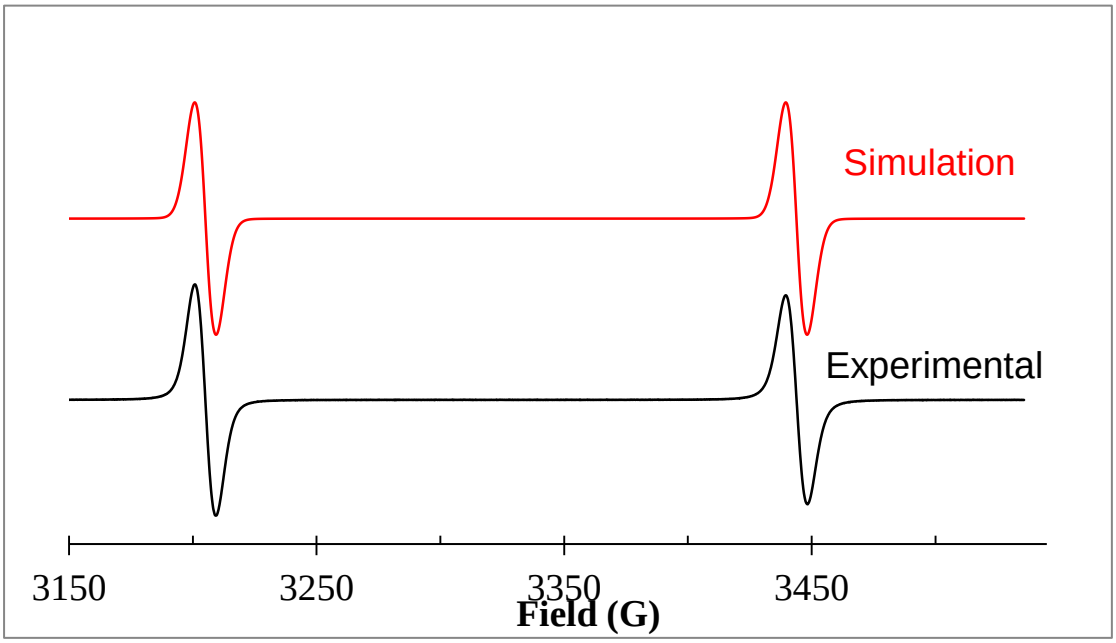
Synthesis of **1**: A mixture of Mes_3P (10 mg, 0.026 mmol) and $B(C_6F_5)_3$ (13.2 mg, 0.026 mmol) was stirring in DCM (2 mL) at room temperature, immediately giving a light purple solution. $(PhCOO)_2$ (3.1 mg, 0.013 mmol) was added to this solution, immediately giving a deep purple solution. The solvent was removed under reduced pressure and the residue was washed with pentane (3 mL), yielding **1** as a deep purple oily solid (21.6 mg, 82%). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ (ppm) -0.9 (bs). ^{31}P NMR (162 MHz, $CDCl_3$): silent.^{19}F NMR (377 MHz, $CDCl_3$): δ (ppm) -133.6 (bs), -160.4 (bs), -166.5 (bs). HRMS (ESI) calcd. for $[PhCOOB(C_6F_5)_3]^-$ 633.0149, found 633.0142;



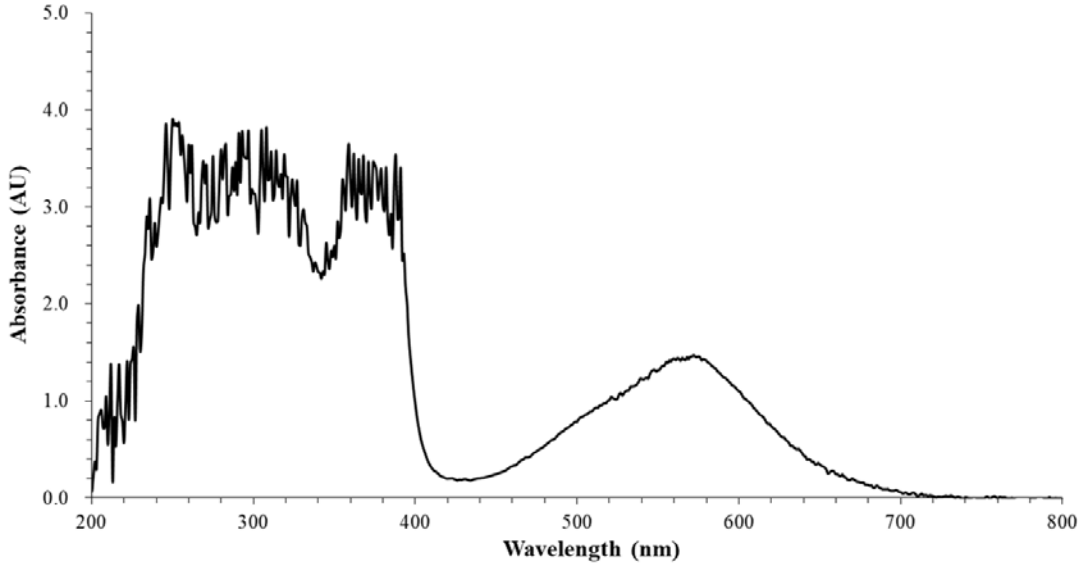
$^{11}B\{^1H\}$ NMR spectrum of **1** (128 MHz, $CDCl_3$)



^{19}F NMR spectrum of **1** (377 MHz, $CDCl_3$).

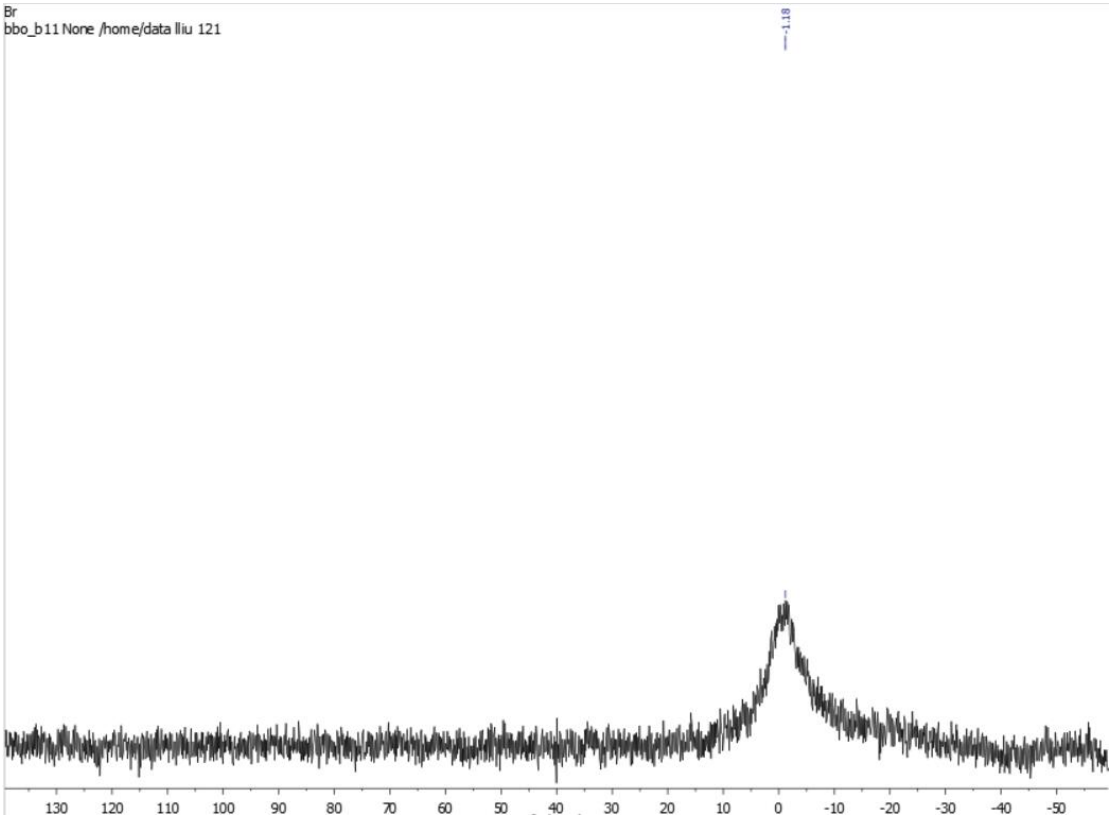


The experimental and simulated X-band EPR spectra of **1** in DCM (g = 2.0085, a_P = 238.7 G).

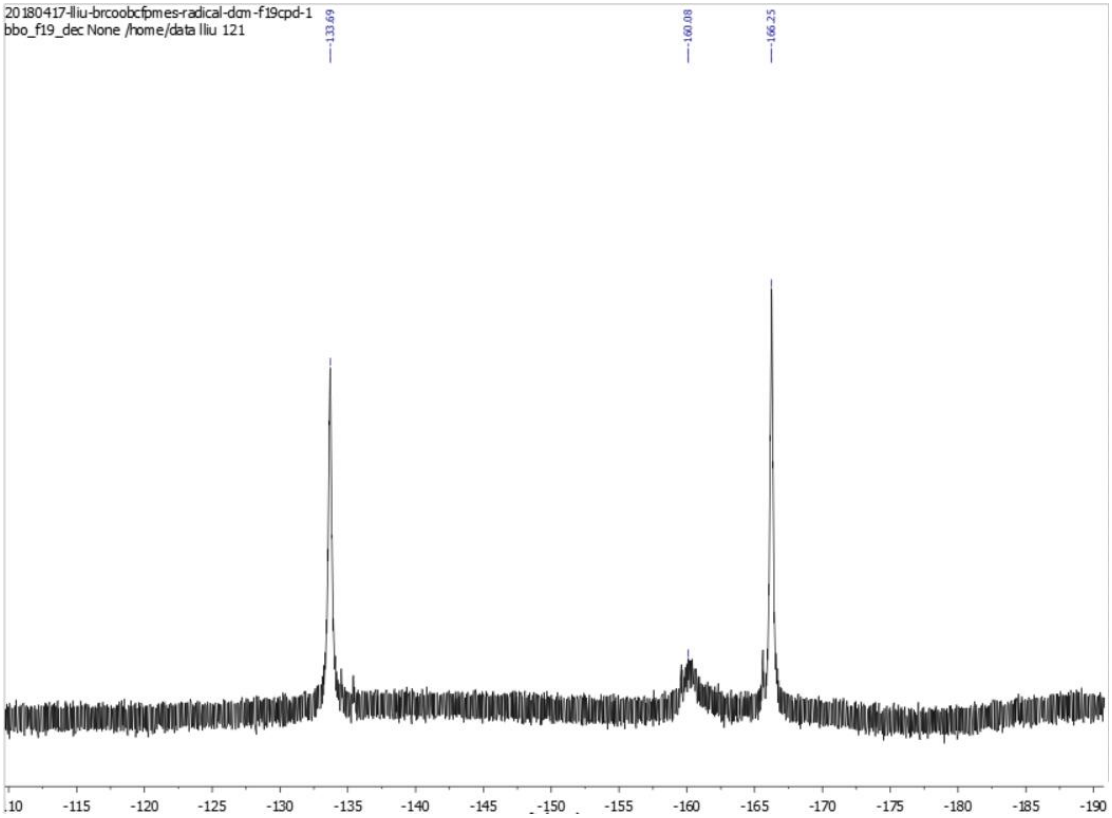


UV-vis study of **1** in C_6H_5Br revealed a visible absorption maximum at 572 nm, in line with the experimental observations of $Mes_3P^{\bullet+}$.

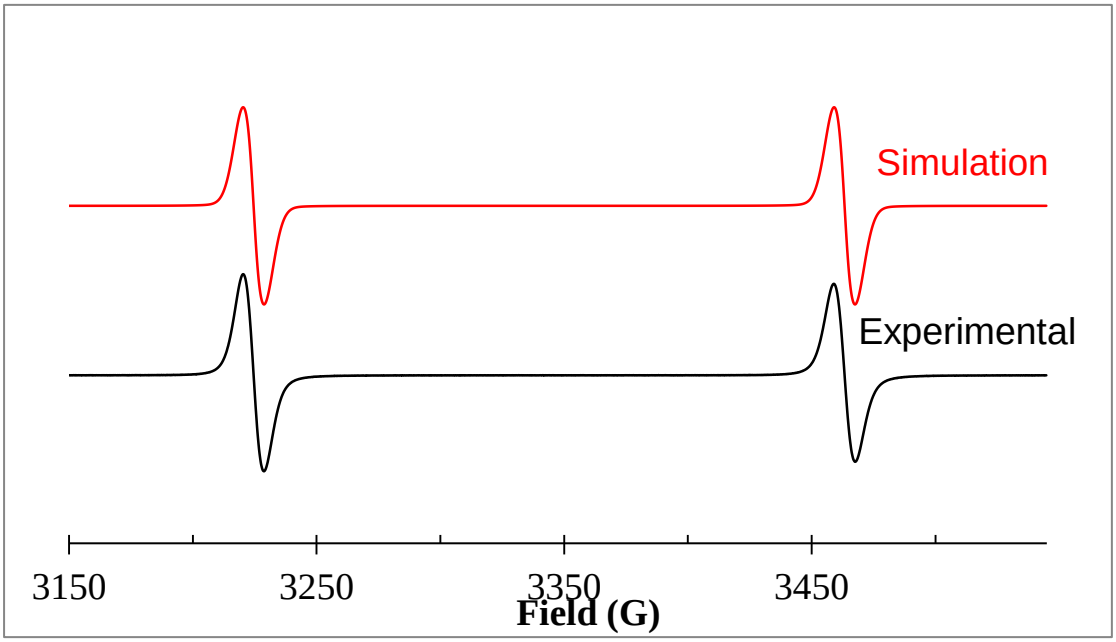
Synthesis of **2**: A mixture of Mes_3P (10 mg, 0.026 mmol) and $B(C_6F_5)_3$ (13.2 mg, 0.026 mmol) was stirring in DCM (2 mL) at room temperature, immediately giving a light purple solution. (*p*-$BrC_6H_4COO)_2$ (5.2 mg, 0.013 mmol) was added to this solution, immediately giving a deep purple solution. The solvent was removed under reduced pressure and the residue was washed with pentane (3 mL), yielding **2** as a deep purple oily solid (22.7 mg, 80%). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ (ppm) -1.2 (bs). ^{31}P NMR (162 MHz, $CDCl_3$): silent.^{19}F NMR (377 MHz, $CDCl_3$): δ (ppm) -133.7 (bs), -160.1 (bs), -166.3 (bs). HRMS (ESI) calcd. for [*p*-$BrC_6H_4COOB(C_6F_5)_3]^-$ 710.9254, found 710.9261.



$^{11}B\{^{1}H\}$ NMR spectrum of **2** (128 MHz, $CDCl_3$)

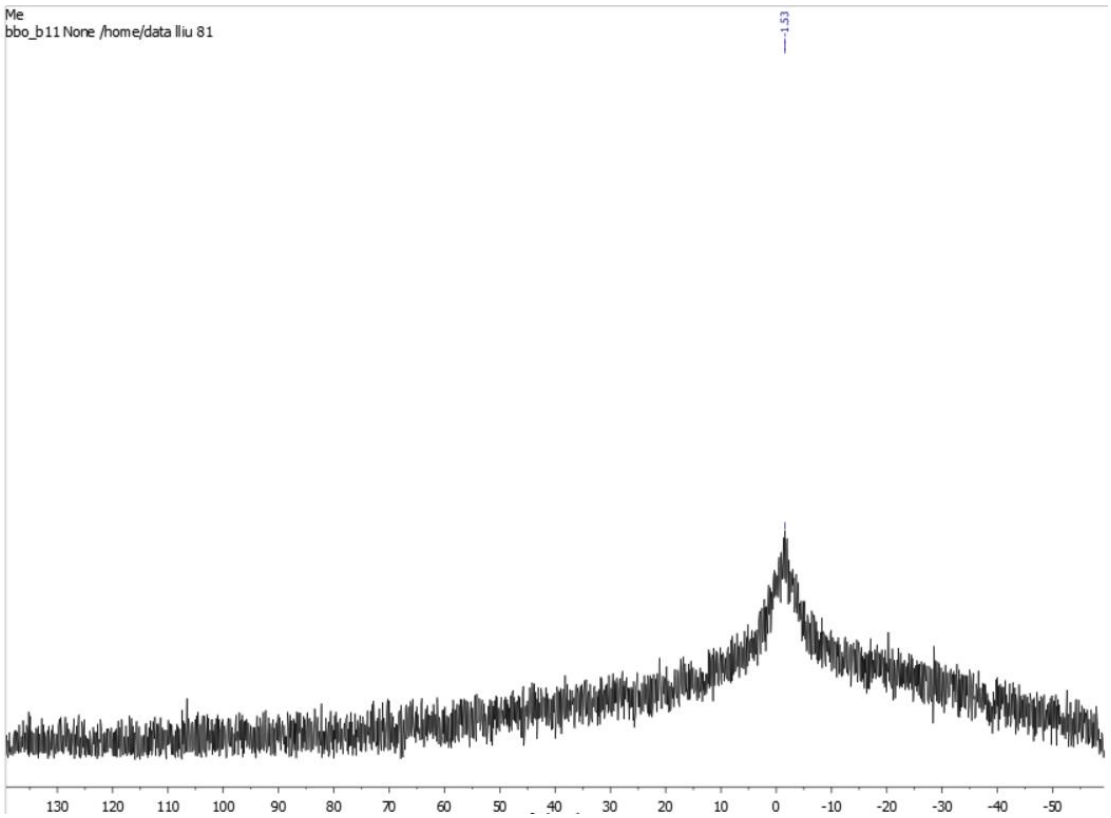


^{19}F NMR spectrum of **2** (377 MHz, $CDCl_3$).

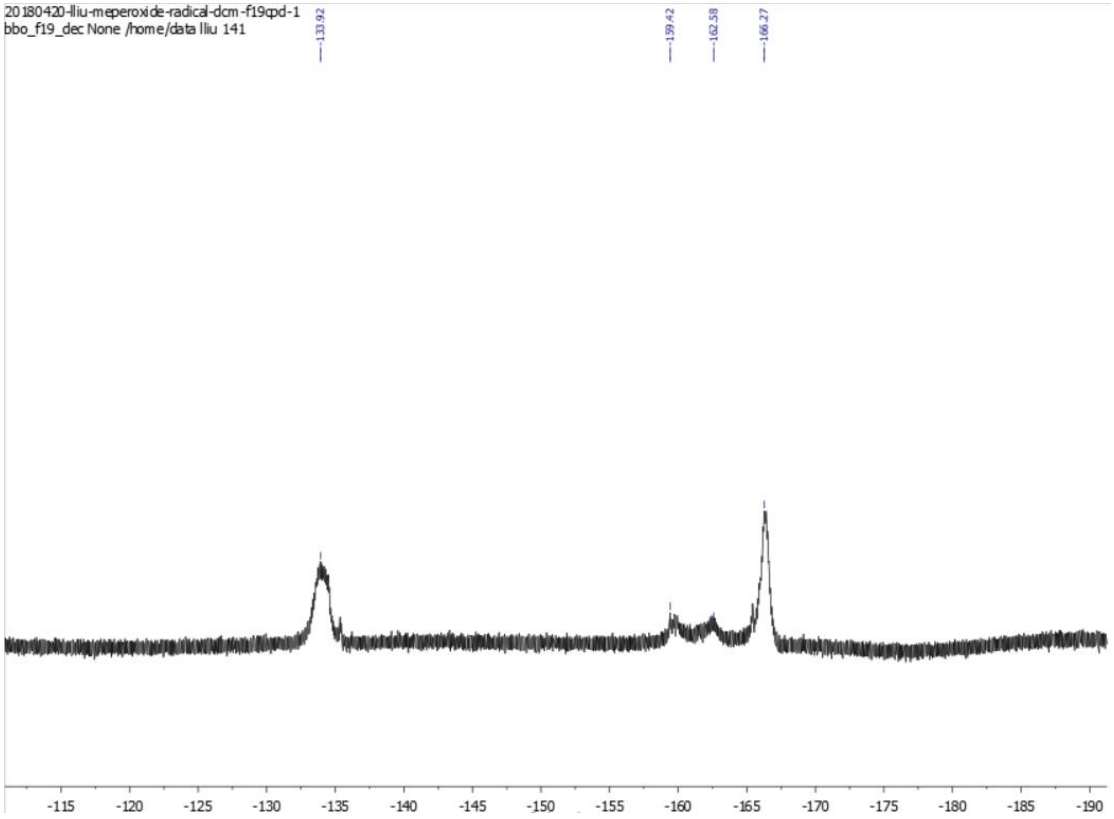


The experimental and simulated X-band EPR spectra of **2** in DCM (g = 2.0092, a_P = 238.7 G).

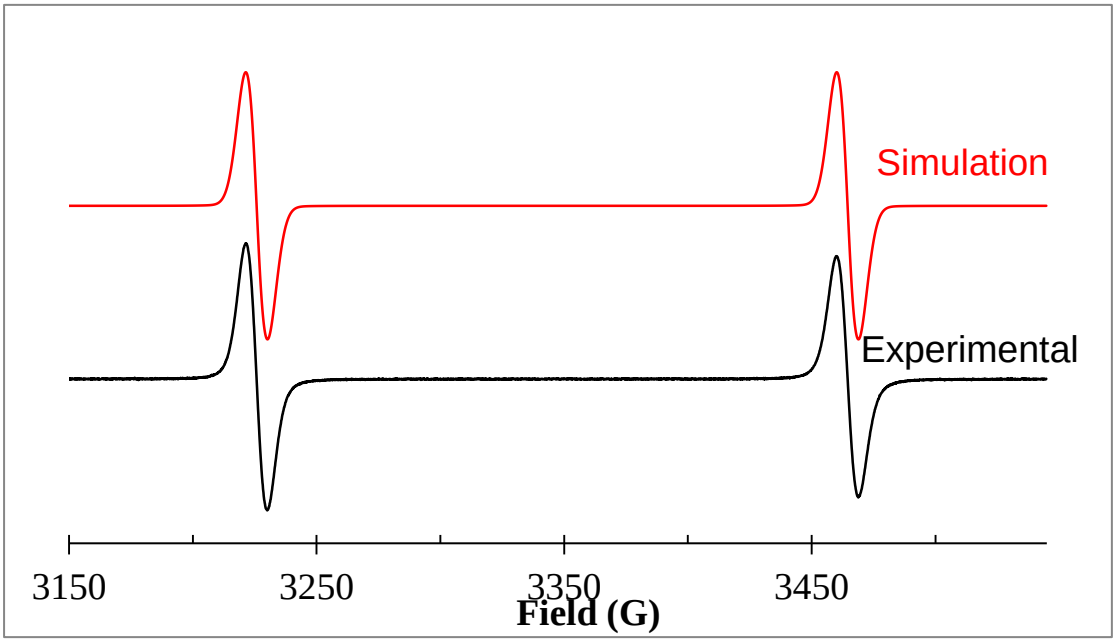
Synthesis of **3**: A mixture of Mes_3P (10 mg, 0.026 mmol) and $B(C_6F_5)_3$ (13.2 mg, 0.026 mmol) was stirring in DCM (2 mL) at room temperature, immediately giving a light purple solution. (*p*-$MeC_6H_4COO)_2$ (3.5 mg, 0.013 mmol) was added to this solution, immediately giving a deep purple solution. The solvent was removed under reduced pressure and the residue was washed with pentane (3 mL), yielding **3** as a deep purple oily solid (20.6 mg, 77%). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ (ppm) -1.5 (bs). ^{31}P NMR (162 MHz, $CDCl_3$): silent.^{19}F NMR (377 MHz, $CDCl_3$): δ (ppm) -133.9 (bs), -159.4 (bs), -162.6 (bs), -166.3 (bs). HRMS (ESI) calcd. for [*p*-$MeC_6H_4COOB(C_6F_5)_3]^-$ 647.0305, found 647.0307.



$^{11}B\{^{1}H\}$ NMR spectrum of **3** (128 MHz, $CDCl_3$)



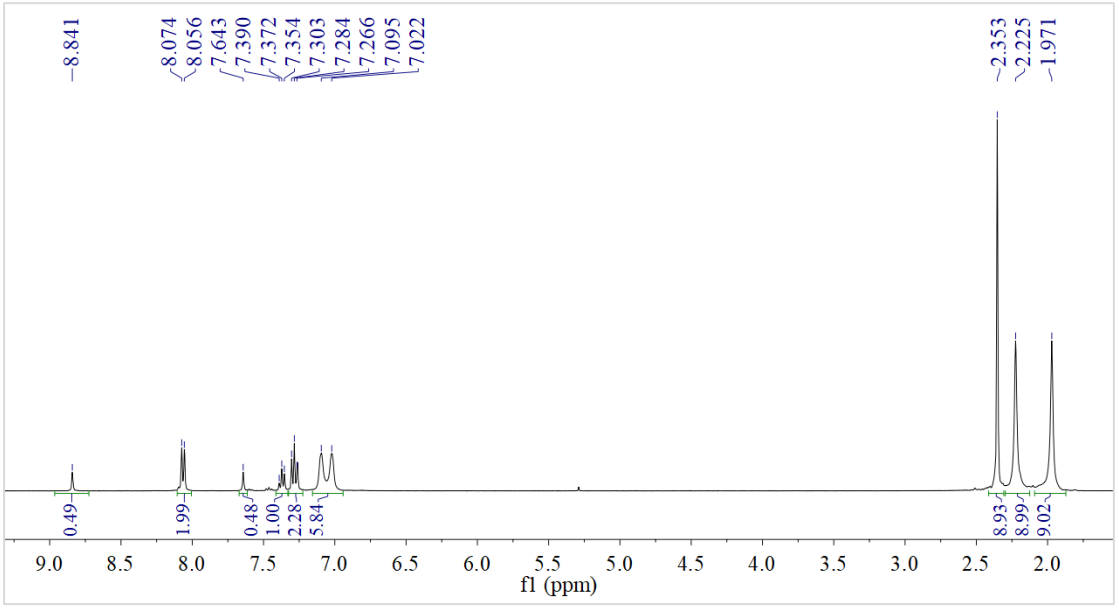
^{19}F NMR spectrum of **3** (377 MHz, $CDCl_3$).



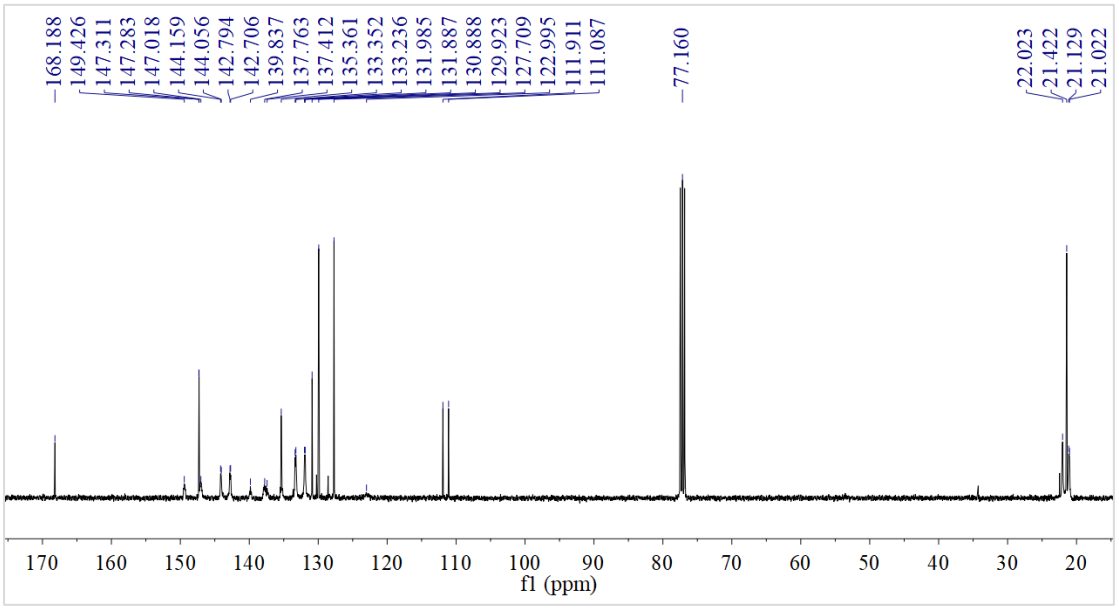
The experimental and simulated X-band EPR spectra of **3** in DCM (g = 2.0089, a_P = 238.7 G).

Synthesis of **10**: Ph_3SnH (6.9 mg, 0.0195 mmol) was added to a DCM (2 mL) solution of **1** (20 mg, 0.0195 mmol) with stirring, immediately giving a light yellow solution. Pentane (5 mL) was added to this solution with stirring and a white precipitate appeared. The solution was decanted and the powder was washed with pentane (2 mL) to give **10** (15.2 mg, 76%). Colorless single crystals were obtained by vapor diffusion of pentane into a saturated DCM solution of **10**. ^{1}H NMR (400 MHz, $CDCl_3$): 8.24 (d, $^1J_{P\text{-}H}$ = 480 Hz, 1H, P*H*), 8.07 (d, $^3J_{H\text{-}H}$ = 7.2 Hz, 2H, Ph-*H*), 7.37 (t, $^3J_{H\text{-}H}$ = 7.2 Hz, 1H, Ph-*H*), 7.28 (t, $^3J_{H\text{-}H}$ = 7.2 Hz, 1H, Ph-*H*), 7.10 (s, 3H, Ar^{Mes}-*H*), 7.02 (s, 3H, Ar^{Mes}-*H*), 2.35 (s, 9H, *Me*), 2.23 (s, 9H, *Me*), 1.97 (s, 9H, *Me*). ^{13}C NMR (100 MHz, $CDCl_3$): 168.2 (carbonyl *C*), 148.2 (d(m), $^1J_{C\text{-}F}$ = 241 Hz, C_6F_5), 147.3 (d, $J_{C\text{-}P}$ = 2.8 Hz, Ar^{Mes}-*C*), 144.1 (d, $J_{C\text{-}P}$ = 10.3 Hz, Ar^{Mes}-*C*), 142.8 (d, $J_{C\text{-}P}$ = 8.8 Hz, Ar^{Mes}-*C*), 138.6 (d(m), $^1J_{C\text{-}F}$ = 243 Hz, C_6F_5), 136.6 (d(m), $^1J_{C\text{-}F}$ = 240 Hz, C_6F_5), 135.4 (s, Ph-*C*), 133.3 (d, $J_{C\text{-}P}$ = 11.6 Hz, Ar^{Mes}-*C*), 131.9 (d, $J_{C\text{-}P}$ = 9.8 Hz, Ar^{Mes}-*C*), 130.9 (s, Ph-*C*), 129.9 (s, Ph-*C*), 127.7 (s, Ph-*C*), 123.0 (m(br), C_6F_5), 11.5 (d, $J_{C\text{-}P}$ = 82.4 Hz, Ar^{Mes}-*C*), 22.0 (br, *Me*), 21.4 (s, *Me*), 21.1 (d(br), $J_{C\text{-}P}$ = 10.7 Hz, *Me*). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ (ppm) -4.5 (s). ^{31}P{^{1}H} NMR (162 MHz,

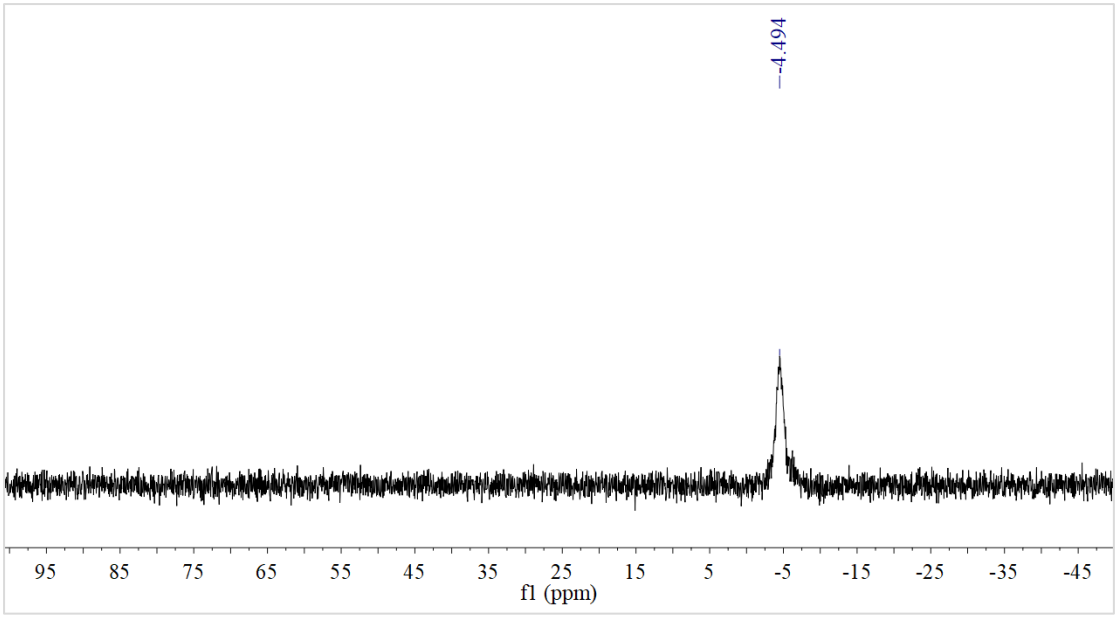
$CDCl_3$): δ (ppm) -27.6 (s). ^{31}P NMR (162 MHz, $CDCl_3$): δ (ppm) -27.6 (d, $^1J_{P-H}$ = 480 Hz). ^{19}F NMR (377 MHz, $CDCl_3$): δ (ppm) -134.2 (d, $^3J_{F-F}$ = 19.2 Hz, 2F, C_6F_5), -162.7 (t, $^3J_{F-F}$ = 20.7 Hz, 1F, C_6F_5), -166.6 (t, $^3J_{F-F}$ = 20.0 Hz, 2F, C_6F_5). HRMS (ESI) calcd. for $C_{27}H_{34}P^+$ 389.2393, found 389.2398; calcd. for $C_{25}H_5BF_{15}O_2^-$ 632.0185, found 632.0179 m/z.



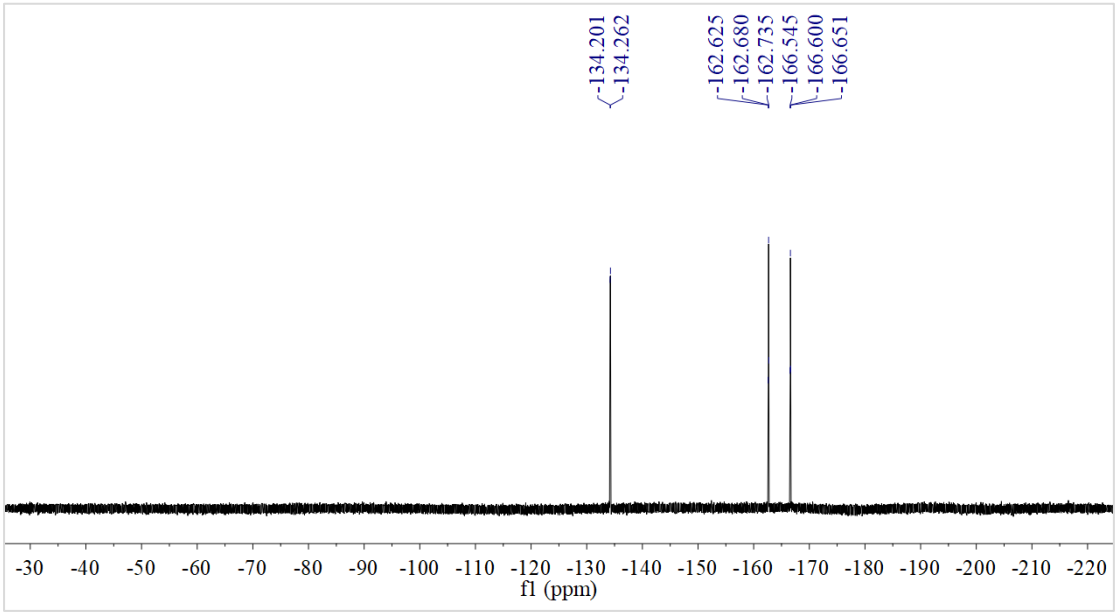
^1H NMR spectrum of **10** (400 MHz, $CDCl_3$).



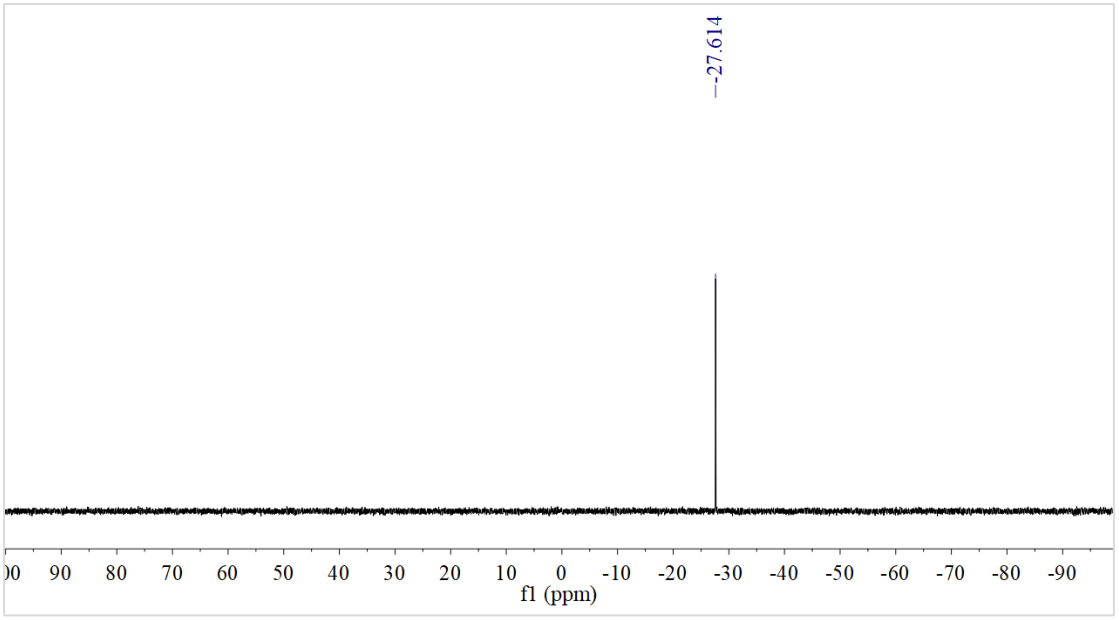
$^{13}C\{^1H\}$ NMR spectrum of **10** (100 MHz, $CDCl_3$).



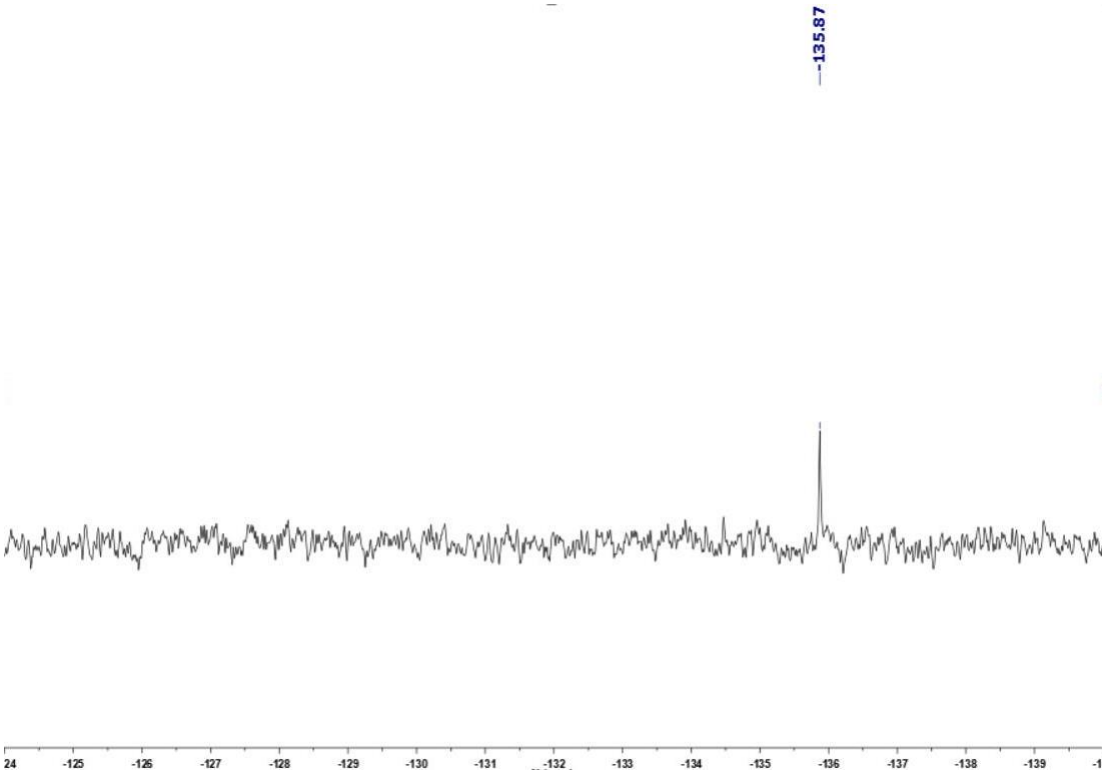
$^{11}B\{^{1}H\}$ NMR spectrum of **10** (128 MHz, $CDCl_3$)



^{19}F NMR spectrum of **10** (377 MHz, $CDCl_3$).



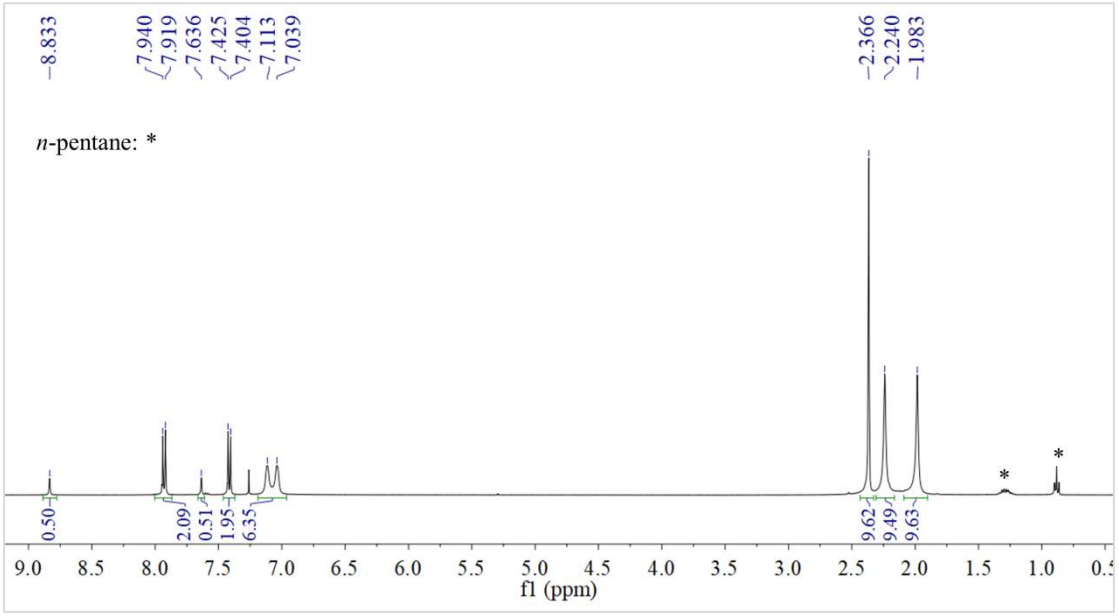
$^{31}P\{^{1}H\}$ NMR spectrum of **10** (162 MHz, $CDCl_3$)



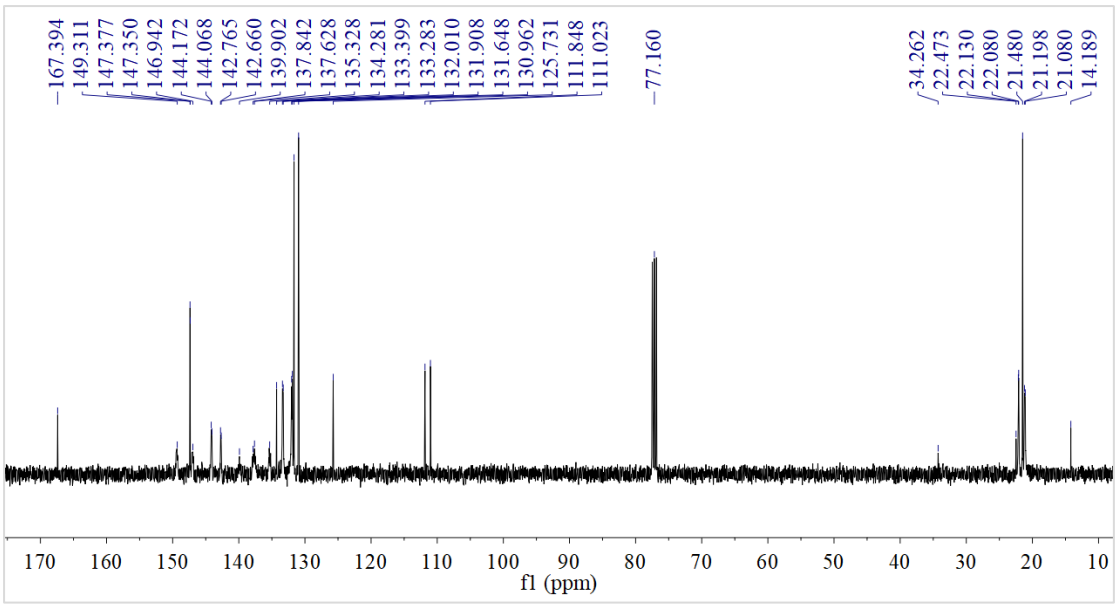
^{119}Sn NMR spectrum of the crude mixture (DCM)

Synthesis of **11**: Ph_3SnH (6.9 mg, 0.0195 mmol) was added to a DCM (2 mL) solution of **2** (20 mg, 0.0195 mmol) with stirring, immediately giving a light yellow solution. Pentane (5 mL) was added to this solution with stirring and a white precipitate appeared. The solution was decanted and the powder was washed with pentane (2 mL)

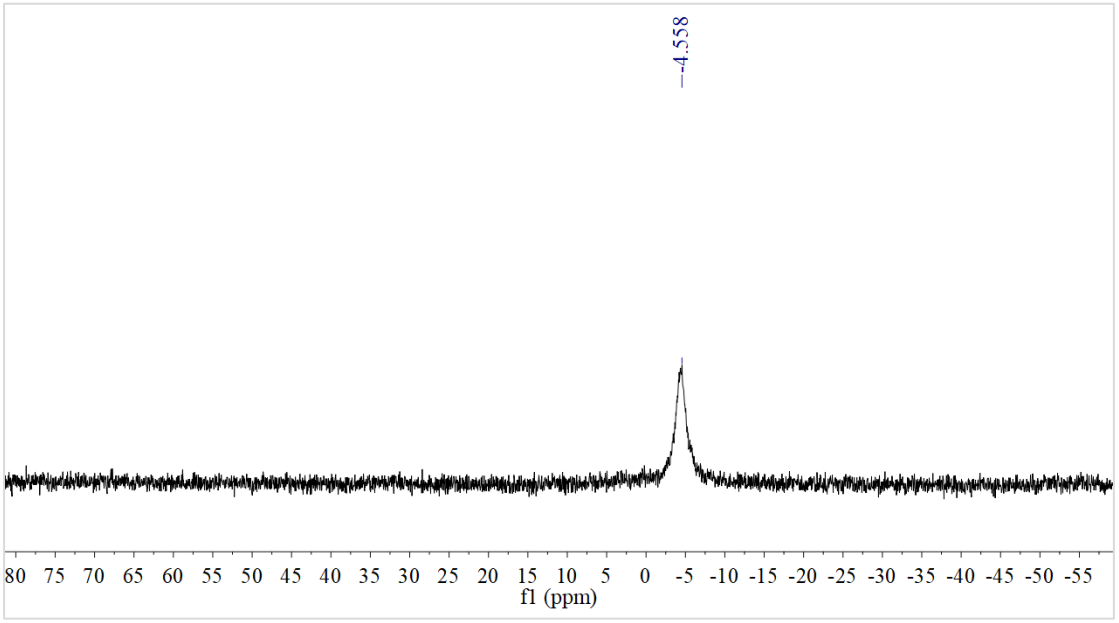
to give **11** (13.3 mg, 62%). Colorless single crystals were obtained by vapor diffusion of pentane into a concentrated 1,2-dichlorobenzene solution of **11**. ^{1}H NMR (400 MHz, $CDCl_3$): 8.23 (d, $^{1}J_{P\text{-}H}$ = 479 Hz, 1H, P*H*), 7.93 (d, $^{3}J_{H\text{-}H}$ = 8.4 Hz, 2H, Ar^{Br}-*H*), 7.41 (d, $^{3}J_{H\text{-}H}$ = 8.4 Hz, 2H, Ar^{Br}-*H*), 7.11 (br, 3H, Ar^{Mes}-*H*), 7.04 (br, 3H, Ar^{Mes}-*H*), 2.37 (s, 9H, *Me*), 2.24 (s, 9H, *Me*), 1.98 (s, 9H, *Me*). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): 167.4 (carbonyl *C*), 148.1 (d(m), $^{1}J_{C\text{-}F}$ = 237 Hz, C_6F_5), 147.4 (d, $J_{C\text{-}P}$ = 2.7 Hz, Ar^{Mes}-*C*), 144.1 (d, $J_{C\text{-}P}$ = 10.4 Hz, Ar^{Mes}-*C*), 142.7 (d, $J_{C\text{-}P}$ = 10.5 Hz, Ar^{Mes}-*C*), 138.9 (d(m), $^{1}J_{C\text{-}F}$ = 206 Hz, C_6F_5), 136.5 (d(m), $^{1}J_{C\text{-}F}$ = 230 Hz, C_6F_5), 134.3 (s, Ar^{Br}-*C*), 133.3 (d, $J_{C\text{-}P}$ = 11.6 Hz, Ar^{Mes}-*C*), 132.0 (d, $J_{C\text{-}P}$ = 10.2 Hz, Ar^{Mes}-*C*), 131.6 (s, Ar^{Br}-*C*), 131.0 (s, Ar^{Br}-*C*), 125.7 (s, Ar^{Br}-*C*), 111.4 (d, $J_{C\text{-}P}$ = 82.5 Hz, Ar^{Mes}-*C*), 22.1 (d(br), $J_{C\text{-}P}$ = 5.0 Hz, *Me*), 21.5 (s, *Me*), 21.1 (d(br), $J_{C\text{-}P}$ = 11.8 Hz, *Me*), 34.3, 22.5, 14.2 (*n*-pentane-*C*). $^{11}B\{^{1}H\}$ NMR (128 MHz, $CDCl_3$): δ (ppm) -4.6 (s). ^{19}F NMR (377 MHz, $CDCl_3$): δ (ppm) -134.4 (d, $^{3}J_{F\text{-}F}$ = 21.1 Hz, 2F, C_6F_5), -162.5 (t, $^{3}J_{F\text{-}F}$ = 20.5 Hz, 1F, C_6F_5), -166.5 (t, $^{3}J_{F\text{-}F}$ = 19.2 Hz, 2F, C_6F_5). $^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$): δ (ppm) -27.6 (s). ^{31}P NMR (162 MHz, $CDCl_3$): δ (ppm) -27.6 (d, $^{1}J_{P\text{-}H}$ = 479 Hz). MS (ESI) Cation: [M+] $C_{27}H_{34}P^{+}$ calc. 389.2393 m/z found 389.2392 m/z; Anion: [M-] $C_{25}H_4BBrF_{15}O_2^{-}$ calc. 709.9290 m/z found 709.9280 m/z.



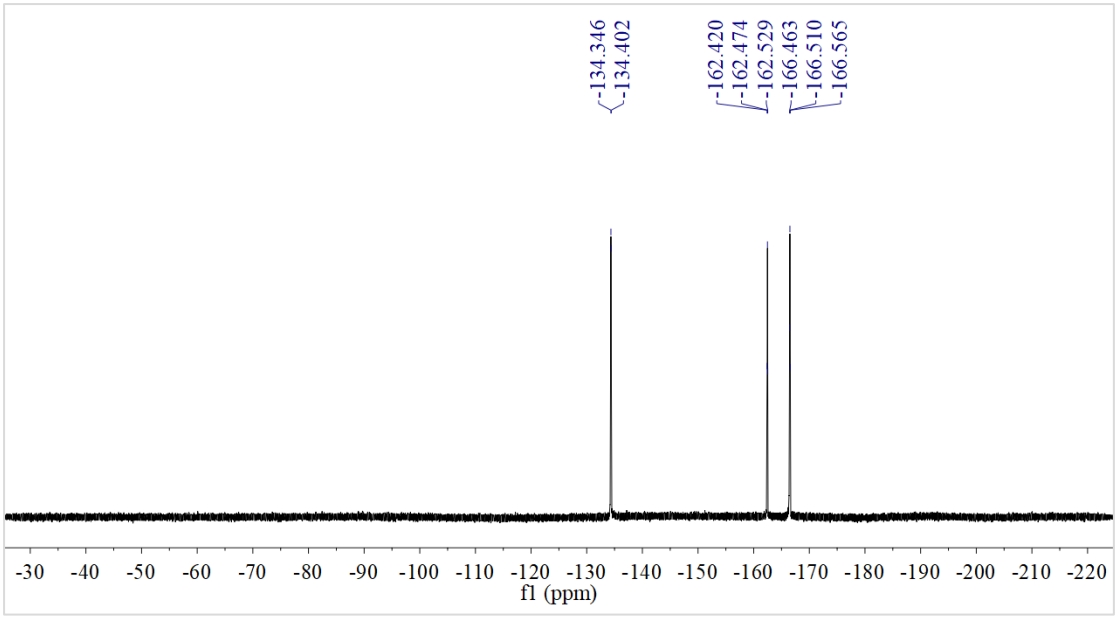
^{1}H NMR spectrum of **11** (400 MHz, $CDCl_3$).



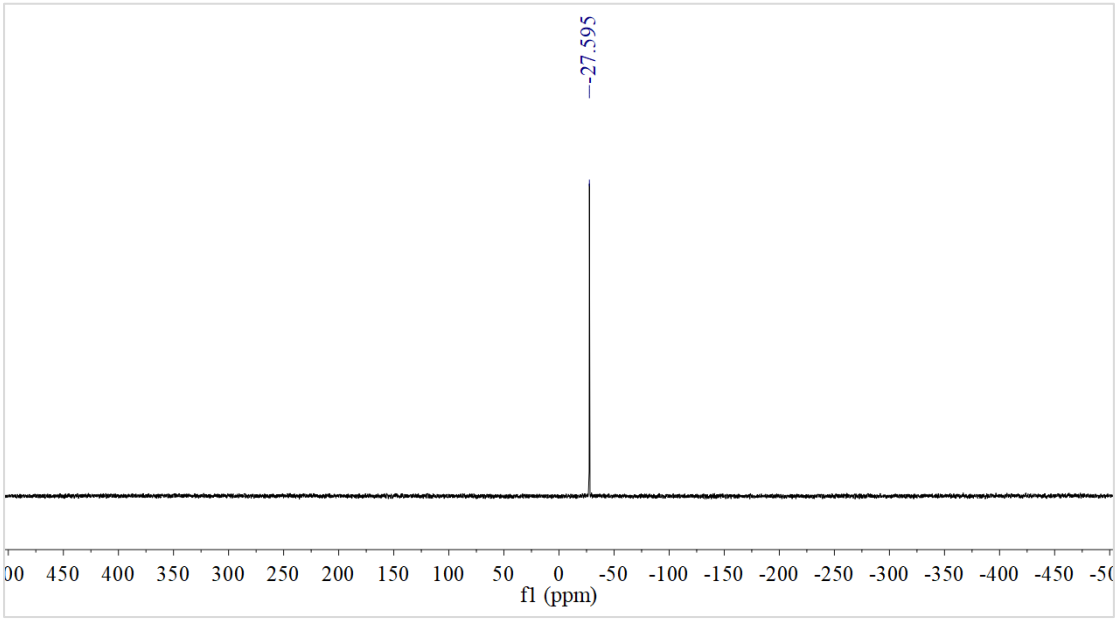
$^{13}C\{^{1}H\}$ NMR spectrum of **11** (100 MHz, $CDCl_3$).



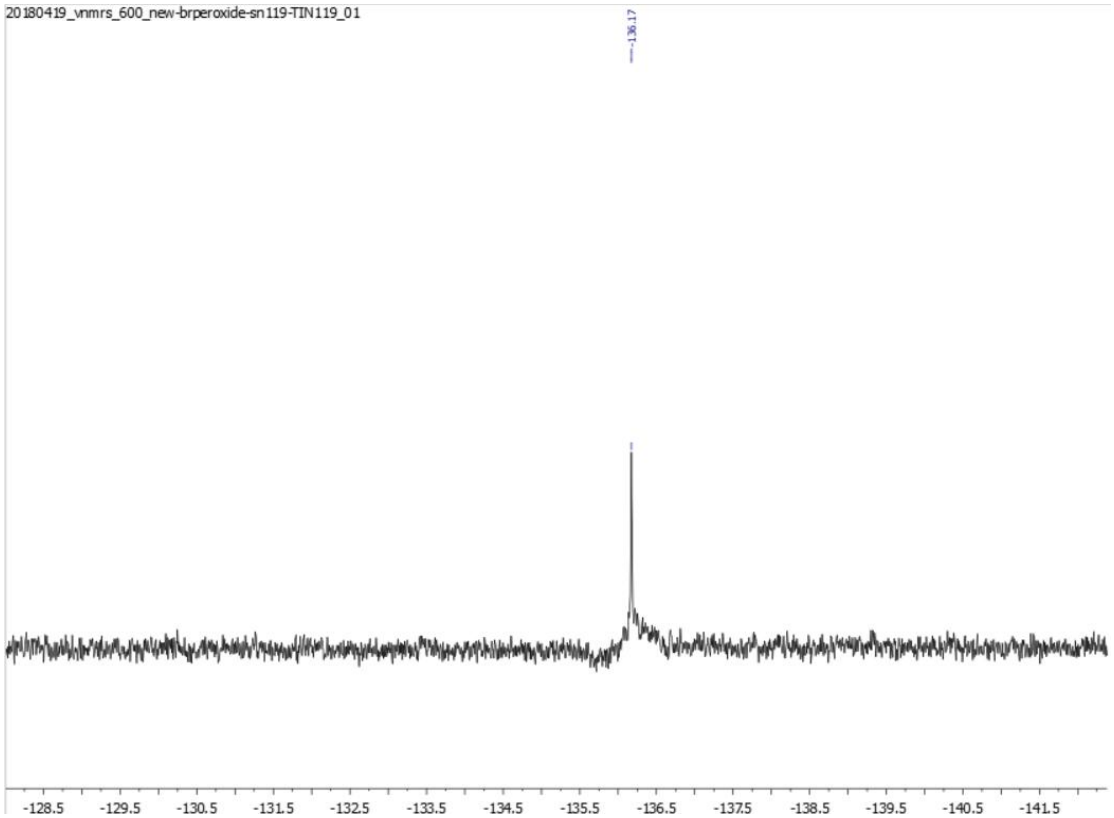
$^{11}B\{^{1}H\}$ NMR spectrum of **11** (128 MHz, $CDCl_3$)



^{19}F NMR spectrum of **11** (377 MHz, $CDCl_3$).



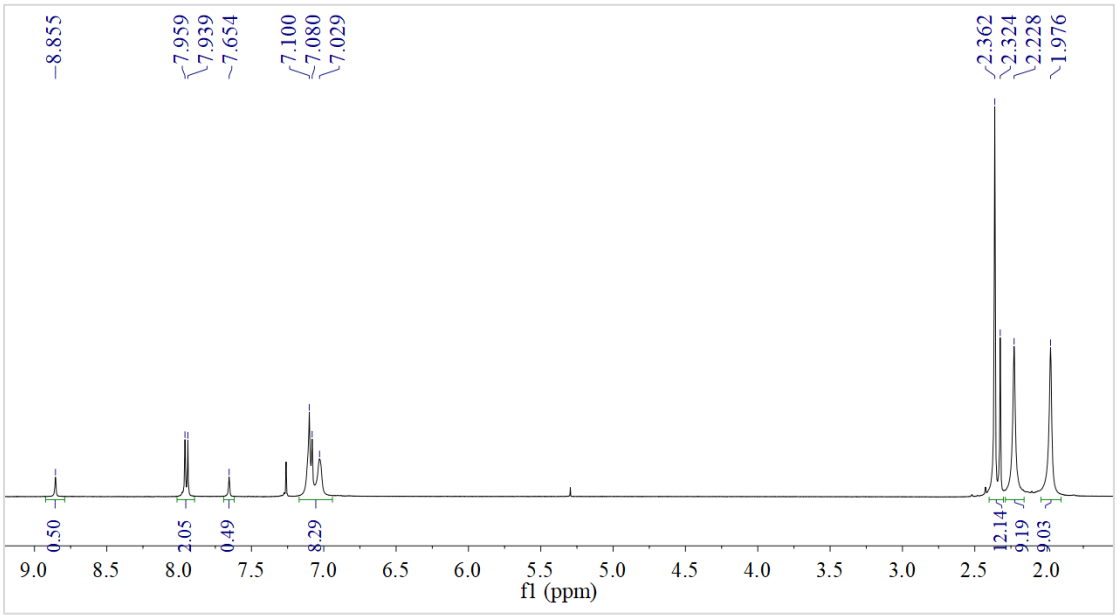
$^{31}P\{^{1}H\}$ NMR spectrum of **11** (162 MHz, $CDCl_3$).



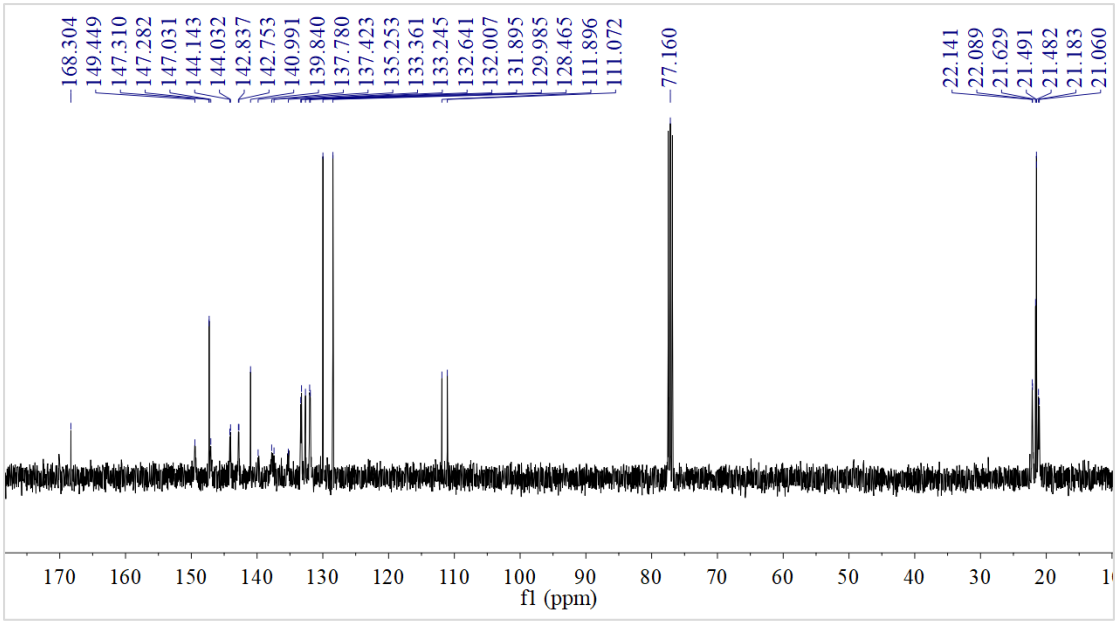
^{119}Sn NMR spectrum of the crude mixture (DCM)

Synthesis of **12**: Ph_3SnH (6.9 mg, 0.0195 mmol) was added to a DCM (2 mL) solution of **3** (20 mg, 0.0195 mmol) with stirring, immediately giving a light yellow solution. Pentane (5 mL) was added to this solution with stirring and a white precipitate appeared. The solution was decanted and the powder was washed with pentane (2 mL) to give **12** (12.5 mg, 62%). Colorless single crystals were obtained by vapor diffusion of pentane into a concentrated 1,2-dichlorobenzene solution of **12**. ^{1}H NMR (400 MHz, $CDCl_3$): 8.25 (d, $^1J_{P\text{-}H}$ = 480 Hz, 1H, P*H*), 7.95 (d, $^3J_{H\text{-}H}$ = 8.0 Hz, 2H, Ar^{tol}-*H*), 7.09 (m, 5H, Ar^{tol}-*H* and Ar^{Mes}-*H*), 7.03 (br, 3H, Ar^{Mes}-*H*), 2.36 (s, 9H, Ar^{Mes}-*Me*), 2.32 (s, 3H, Ar^{tol}-*Me*), 2.23 (s, 9H, Ar^{Mes}-*Me*), 1.98 (s, 9H, Ar^{Mes}-*Me*). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): 168.3 (carbonyl *C*), 148.2 (d(m), $^1J_{C\text{-}F}$ = 242 Hz, C_6F_5), 147.4 (d, $J_{C\text{-}P}$ = 2.8 Hz, Ar^{Mes}-*C*), 144.1 (d, $J_{C\text{-}P}$ = 11.1 Hz, Ar^{Mes}-*C*), 142.8 (d, $J_{C\text{-}P}$ = 8.4 Hz, Ar^{Mes}-*C*), 141.0 (s, Ar^{tol}-*C*), 138.8 (d(m), $^1J_{C\text{-}F}$ = 206 Hz, C_6F_5), 136.3 (d(m), $^1J_{C\text{-}F}$ = 217 Hz, C_6F_5), 133.3 (d, $J_{C\text{-}P}$ = 11.6 Hz, Ar^{Mes}-*C*), 132.6 (s, Ar^{tol}-*C*), 131.9 (d, $J_{C\text{-}P}$ = 11.2 Hz, Ar^{Mes}-*C*), 130.0 (s, Ar^{tol}-*C*), 128.5 (s, Ar^{tol}-*C*), 111.5 (d, $J_{C\text{-}P}$

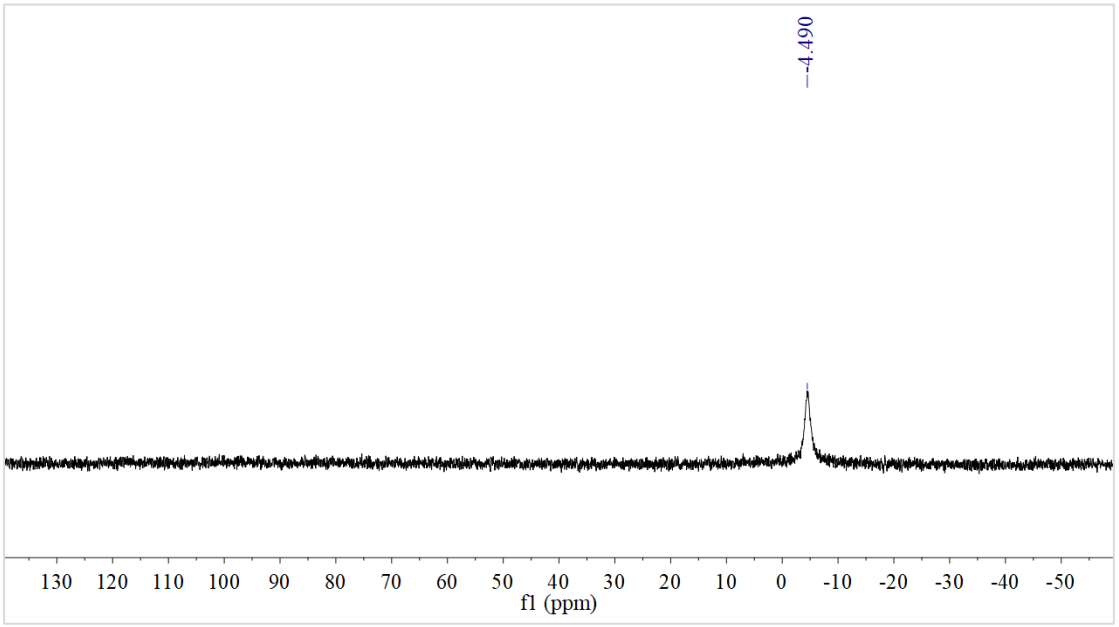
= 82.4 Hz, Ar^{Mes}-*C*), 22.1 (d(br), $J_{C\text{-}P}$ = 5.2 Hz, Ar^{Mes}-*Me*), 21.6 (s, Ar^{tol}-*Me*), 21.5 (d, $J_{C\text{-}P}$ = 0.9 Hz, Ar^{Mes}-*Me*), 21.1 (d(br), $J_{C\text{-}P}$ = 12.3 Hz, Ar^{Mes}-*Me*). $^{11}B\{^{1}H\}$ NMR (128 MHz, $CDCl_3$): δ (ppm) -4.5 (s). ^{19}F NMR (377 MHz, $CDCl_3$): δ (ppm) -134.1 (d, $^{3}J_{F\text{-}F}$ = 22.8 Hz, 2F, C_6F_5), -162.8 (t, $^{3}J_{F\text{-}F}$ = 20.9 Hz, 1F, C_6F_5), -166.7 (t, $^{3}J_{F\text{-}F}$ = 19.0 Hz, 2F, C_6F_5). $^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$): δ (ppm) -27.6 (s). ^{31}P NMR (162 MHz, $CDCl_3$): δ (ppm) -27.6 (d, $^{1}J_{P\text{-}H}$ = 480 Hz). MS (ESI) Cation: [M+] $C_{27}H_{34}P^{+}$ calc. 389.2393 m/z found 389.2393 m/z; Anion: [M-] $C_{26}H_7BF_{15}O_2^{-}$ calc. 646.0341 m/z found 646.0334 m/z.



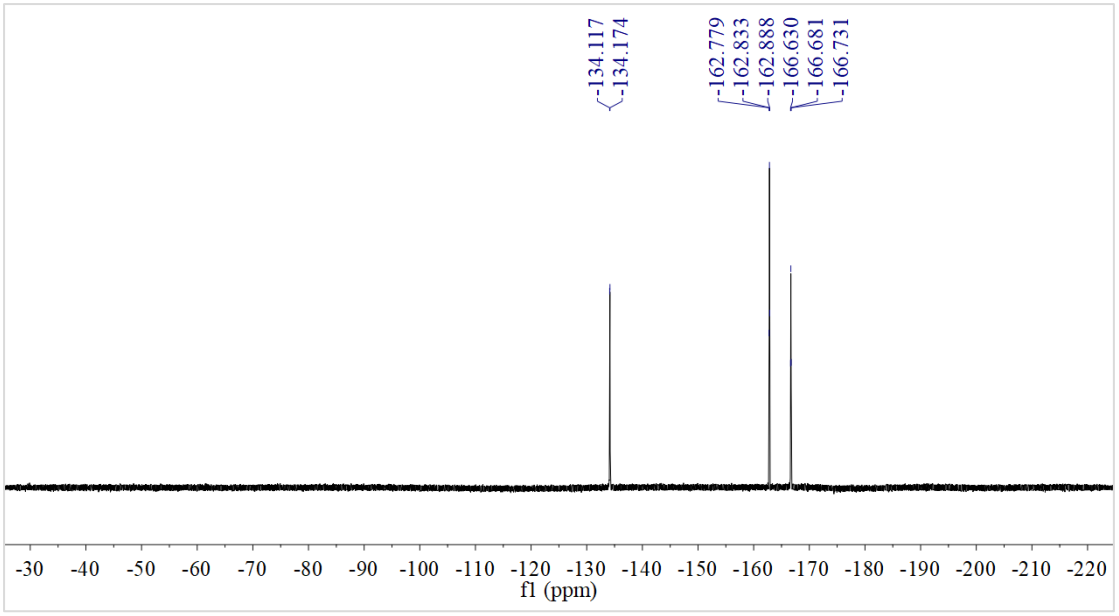
^{1}H NMR spectrum of **12** (400 MHz, $CDCl_3$).



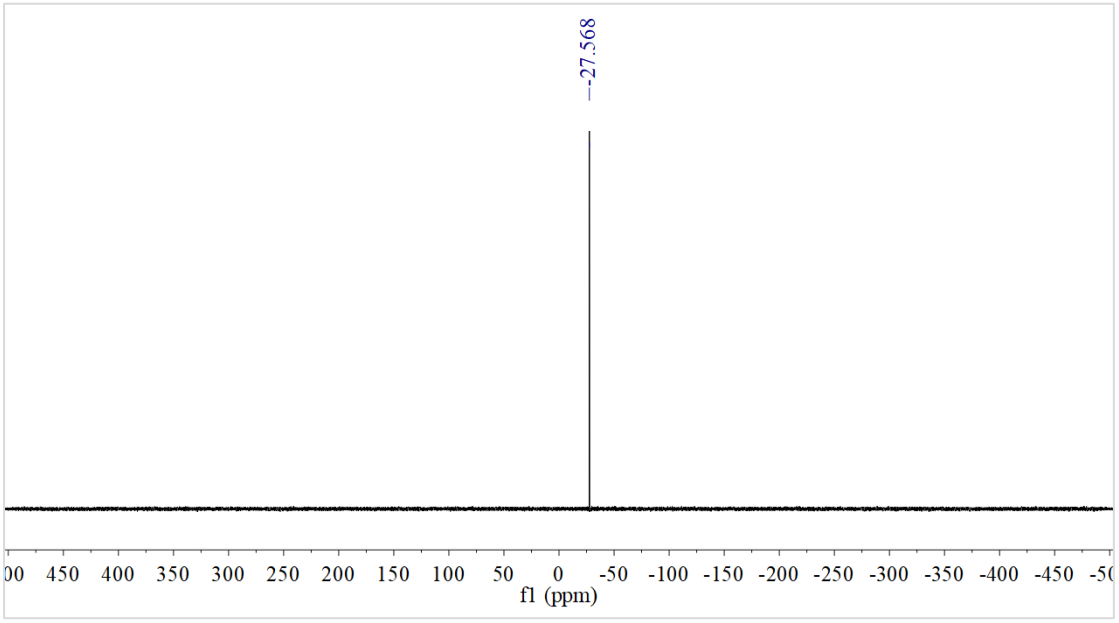
$^{13}C\{^{1}H\}$ NMR spectrum of **12** (100 MHz, $CDCl_3$).



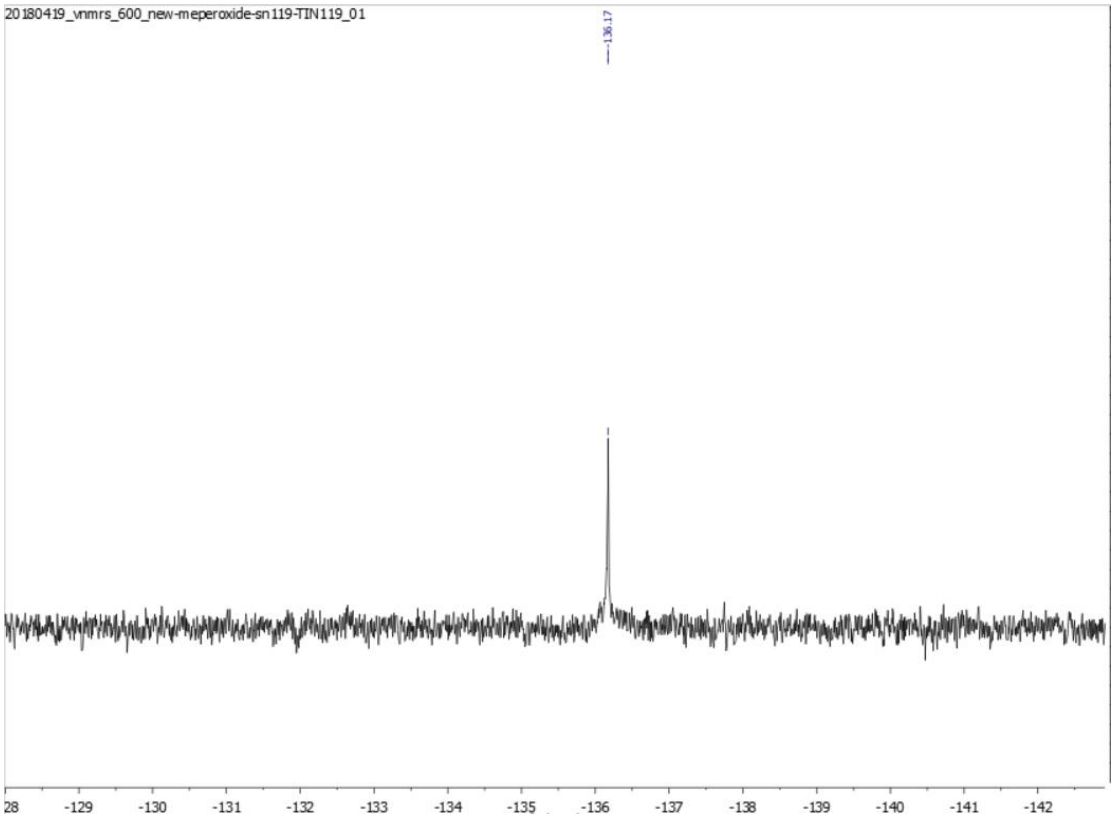
$^{11}B\{^{1}H\}$ NMR spectrum of **12** (128 MHz, $CDCl_3$)



^{19}F NMR spectrum of **12** (377 MHz, $CDCl_3$).

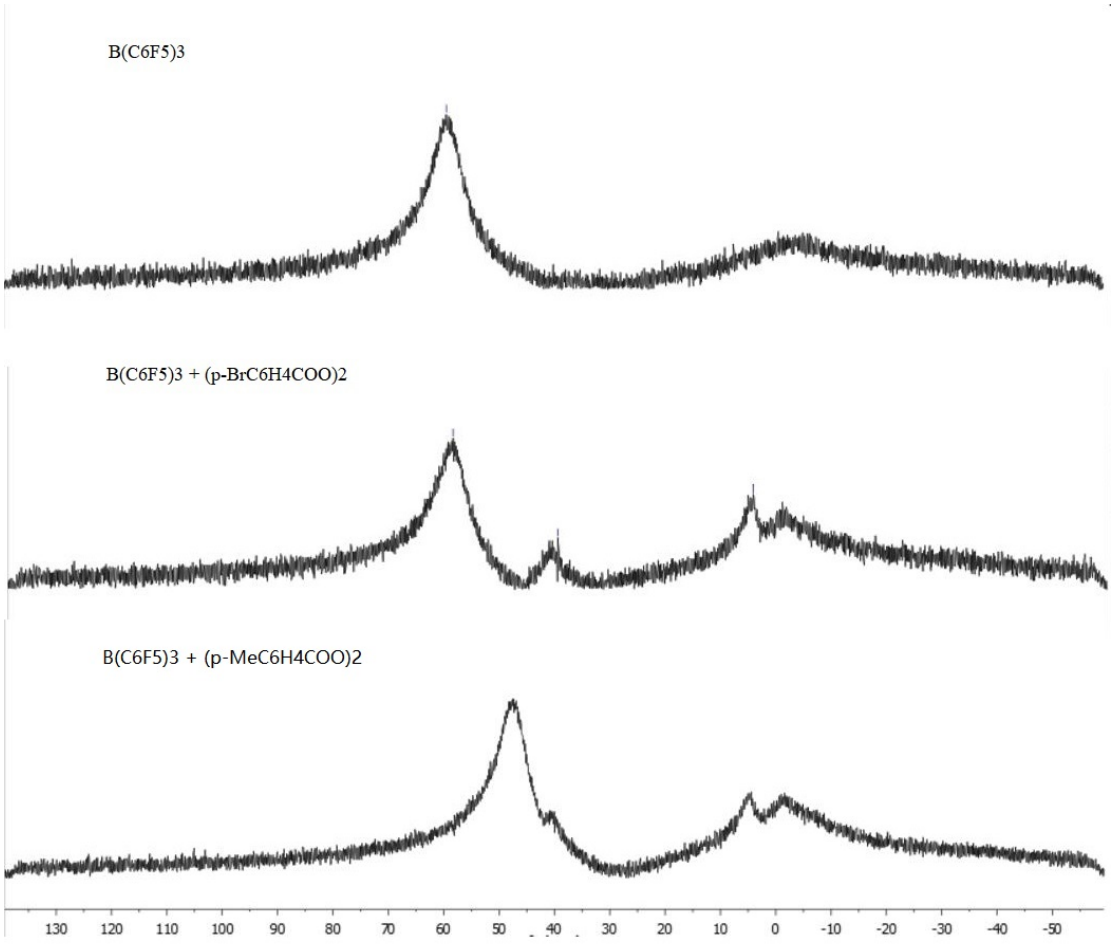


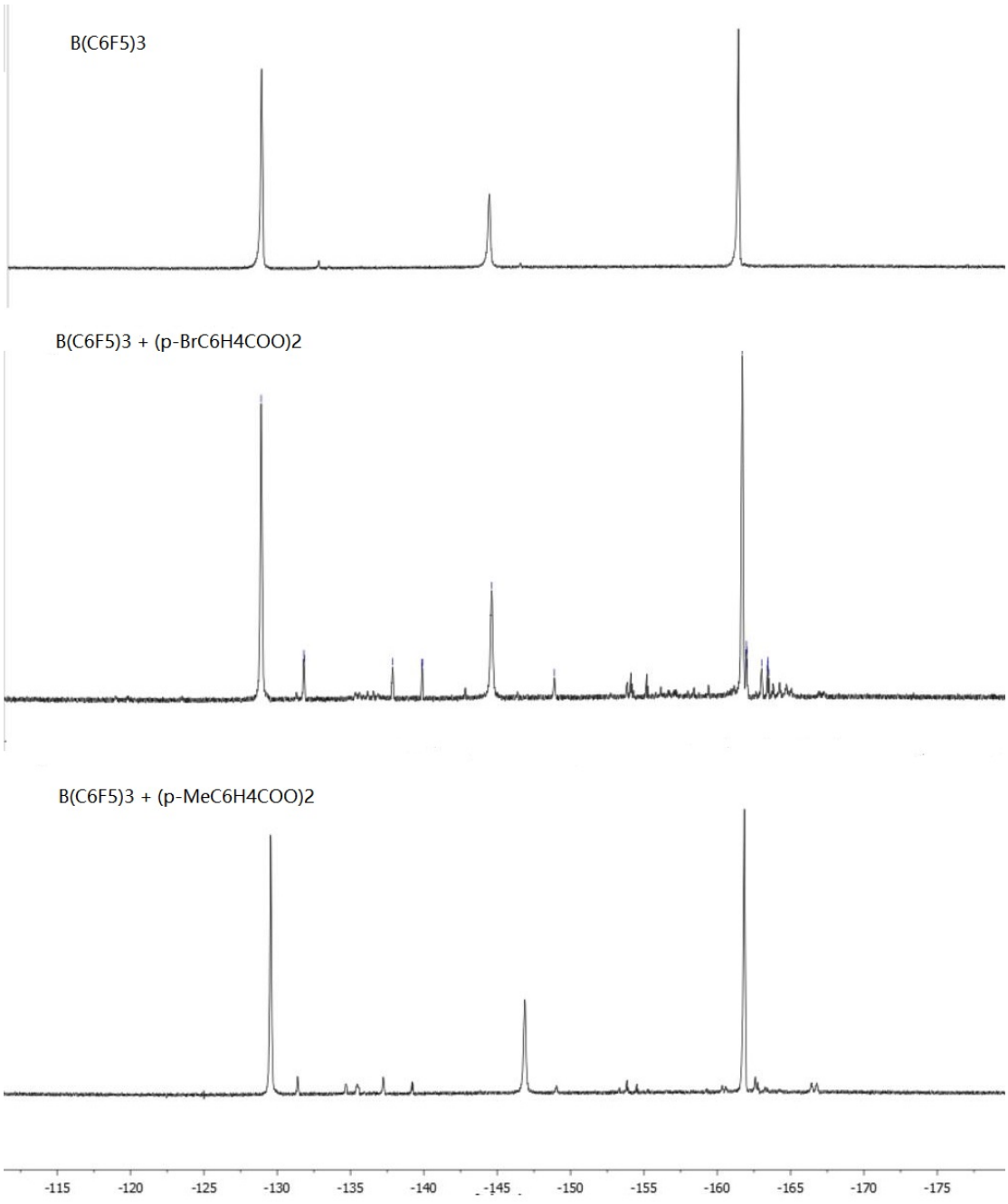
$^{31}P\{^{1}H\}$ NMR spectrum of **12** (162 MHz, $CDCl_3$).



^{119}Sn NMR spectrum of the crude mixture (DCM)

^{11}B and ^{19}F NMR spectra revealing interaction of peroxides with $B(C_6F_5)_3$ in solution




B(C6F5)3
B(C6F5)3 + (p-BrC6H4COO)2
B(C6F5)3 + (p-MeC6H4COO)2
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
-175

Details of Single Crystal X-ray Diffraction Study:

X-ray Data Collection and Reduction. Crystals were coated in Paratone-N oil in an N_2 filled glovebox, mounted on a MiTegen Micromount, and placed under a N_2 stream, thus maintaining a dry, O_2-free environment for each crystal. The data were collected on a Bruker Apex II diffractometer using a graphite monochromator with Mo Kα radiation (λ = 0.71073 Å). The data were collected at 150(2) K for all crystals. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. Data were corrected for absorption effects using the empirical multiscan method (SADABS).

Structure Solution and Refinement. The structures were solved by direct methods using XS and subjected to full-matrix least-squares refinement on F^2 using XL as implemented in the SHELXTL suite of programs. All non-hydrogen atoms were refined with anisotropically thermal parameters. Carbon bound hydrogen atoms were placed in geometrically calculated positions and refined using an appropriate riding model and coupled isotropic thermal parameters.

Table S1. Summary of crystallographic data for compound **10-12.**

	10	**11**	**12**
empirical formula	C52 H39 B F15 O2 P	C52 H38 B Br F15 O2 P	C53 H41 B F15 O2 P
formula weight	1022.61	1101.50	1036.64
crystal system	Monoclinic	Triclinic	Monoclinic
space group	P 21/n	$P\bar{1}$	P 21/c
a (Å)	13.040(4)	12.6688(9)	12.4203(12)
b (Å)	17.682(6)	18.7187(14)	20.1153(17)
c (Å)	20.467(7)	20.0531(14)	18.9334(18)
α (deg.)	90	90.811(3)	90
β (deg.)	99.613(7)	91.169(3)	97.534(3)
γ (deg.)	90	97.947(3)	90
vol ($Å^3$)	4653(3)	4708.1(6)	4689.5(7)
Z	4	4	4
μ (mm^{-1})	0.161	1.009	0.161
F(000)	2088.0	2224.0	2120.0
T(K)	150	150	150
reflections collected	9152	19418	9726
R_{int}	0.0804	0.1288	0.1297
GOF(F^2)	0.996	0.982	1.040
R1 indices [I>2σ(I)]	0.0589	0.0636	0.0512
wR2 indices (all data)	0.1762	0.1642	0.1513
CCDC No.	1826281	1839053	1839054

Computational Details

Calculations were carried out with the Gaussian 09 package.[S2] Geometry optimizations were performed with the M06 functional.[S3] The Def2-SVP basis set was used for all the atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide Gibbs free energies. All the solution-phase free energies reported in the paper correspond to the reference state of 1 mol/L, 298K.

Energies of Optimized Structures:

	Free Energies (Hartree)
$B(C_6F_5)_3$	-2205.592543
$(PhCOO)_2$	-838.994467
$(p\text{-}BrC_6H_4COO)_2$	-5985.324365
$(p\text{-}MeC_6H_4COO)_2$	-917.460615
$(PhCOO)_2$• $B(C_6F_5)_3$	-3044.593676
$(p\text{-}BrC_6H_4COO)_2$• $B(C_6F_5)_3$	-8190.920981
$(p\text{-}MeC_6H_4COO)_2$• $B(C_6F_5)_3$	-3123.061453
$(PhCOO)_2$• $2B(C_6F_5)_3$	-5250.175575
$(p\text{-}BrC_6H_4COO)_2$• $2B(C_6F_5)_3$	-10396.503110
$(p\text{-}MeC_6H_4COO)_2$• $2B(C_6F_5)_3$	-5328.646933

Cartesian Coordinates:

$B(C_6F_5)_3$

5	8.172881	-1.178119	1.636668
6	7.917447	-0.320122	0.347302
6	8.644407	-0.515814	-0.830646
6	6.953439	0.692016	0.318332
6	8.440465	0.248066	-1.974516

6	6.707019	1.463157	-0.811899
6	7.461882	1.239904	-1.961928
6	8.380117	-2.725932	1.518040
6	9.224300	-3.433216	2.385442
6	7.734921	-3.489439	0.535527
6	9.436854	-4.802634	2.281648
6	7.908568	-4.863957	0.413587
6	8.769037	-5.519802	1.290958
6	8.213898	-0.469787	3.033781
6	8.718944	0.826983	3.194181
6	7.739111	-1.089939	4.196727
6	8.757532	1.474282	4.424340
6	7.744201	-0.468112	5.439606
6	8.262238	0.820997	5.550787
9	8.285636	1.419560	6.718413
9	9.254603	2.688615	4.536555
9	9.213303	1.486080	2.158156
9	7.239104	-2.313889	4.139885
9	7.274070	-1.079711	6.507063
9	9.881559	-2.799188	3.342630
9	10.253314	-5.427666	3.104715
9	8.949067	-6.814867	1.185506
9	7.273383	-5.547662	-0.515509
9	6.896249	-2.918402	-0.313727
9	9.587751	-1.444914	-0.882161
9	9.158643	0.047590	-3.060668
9	7.251054	1.967055	-3.034919
9	5.778870	2.398113	-0.806889
9	6.217020	0.936920	1.392702

$(PhCOO)_2$

8	-0.677124	0.825851	-1.412923
8	1.485025	0.944832	-1.594924
6	0.241348	1.542095	-1.681054
6	0.115279	2.950164	-2.126944
6	-1.010287	3.640670	-1.660031
1	-1.682004	3.140844	-0.956818
6	0.965896	3.559654	-3.057463
1	1.833888	3.023365	-3.444157
6	-1.262501	4.938332	-2.087253
1	-2.133302	5.478764	-1.706485
6	0.694644	4.849592	-3.500307
1	1.355625	5.319137	-4.233698
6	-0.409680	5.543062	-3.009440
1	-0.610107	6.562301	-3.352215
8	2.558922	1.883304	-1.560315
6	3.620965	1.472526	-0.776951
8	4.385052	2.341057	-0.475774
6	3.780705	0.043327	-0.417606
6	4.497216	-0.212889	0.758626
6	3.378245	-1.024140	-1.229579
6	4.778990	-1.519486	1.136907
6	3.684135	-2.328947	-0.857882
6	4.373875	-2.579038	0.326818
1	2.834194	-0.835696	-2.156712
1	3.377294	-3.159363	-1.499429
1	4.601708	-3.608527	0.618026
1	5.325091	-1.713321	2.064075
1	4.829246	0.631799	1.368367

$(p\text{-}BrC_6H_4COO)_2$

8	-0.655147	0.809944	-1.451841
8	1.504508	0.929409	-1.667317
6	0.259731	1.528974	-1.723161
6	0.127611	2.943660	-2.143153
6	-1.004266	3.617937	-1.667689
1	-1.677838	3.101277	-0.978658
6	0.974538	3.581139	-3.058221
1	1.847901	3.063472	-3.457621
6	-1.269961	4.921883	-2.061791
1	-2.143569	5.455445	-1.679294
6	0.702529	4.877653	-3.476890
1	1.355238	5.375957	-4.197910
6	-0.410134	5.544313	-2.966482
8	2.580970	1.864097	-1.631623
6	3.631439	1.462783	-0.827271
8	4.394934	2.332620	-0.529921
6	3.780233	0.040242	-0.440546
6	4.497607	-0.197879	0.738929
6	3.370346	-1.043766	-1.226414
6	4.772416	-1.493756	1.152480
6	3.662187	-2.343606	-0.831615
6	4.350844	-2.561383	0.360718
1	2.827908	-0.878136	-2.158625
1	3.353521	-3.192129	-1.446899
1	5.318788	-1.681234	2.079997
1	4.839817	0.655133	1.331161
35	4.723365	-4.327007	0.908386
35	-0.762737	7.314610	-3.512356

$(p\text{-}MeC_6H_4COO)_2$

8	-0.669413	0.831391	-1.415021
8	1.491128	0.944276	-1.615631
6	0.248515	1.547413	-1.689114
6	0.122780	2.954468	-2.129686
6	-1.011752	3.640613	-1.678457
1	-1.692226	3.137295	-0.986129
6	0.979759	3.582992	-3.041634
1	1.860130	3.061722	-3.420578
6	-1.262752	4.938330	-2.099566
1	-2.141414	5.471591	-1.721729
6	0.705059	4.872982	-3.476042
1	1.379064	5.353082	-4.193203
6	-0.411272	5.576599	-3.009747
8	2.569787	1.876798	-1.574226
6	3.620896	1.466182	-0.774605
8	4.379577	2.337136	-0.463855
6	3.776792	0.039651	-0.413512
6	4.498971	-0.221272	0.757462
6	3.366464	-1.035072	-1.212882
6	4.775957	-1.526849	1.137715
6	3.670491	-2.335946	-0.835497
6	4.371734	-2.607530	0.345763
1	2.814259	-0.854978	-2.136753
1	3.350658	-3.168415	-1.471265
1	5.323794	-1.717296	2.066544
1	4.837883	0.621016	1.366866
6	4.701774	-4.014427	0.730955
1	3.881091	-4.705370	0.483145
1	5.595087	-4.371030	0.189433

1	4.915252	-4.102964	1.806579
6	-0.703875	6.961315	-3.493451
1	0.217193	7.507035	-3.749002
1	-1.327888	6.937024	-4.403831
1	-1.254866	7.546203	-2.741362

$(PhCOO)_2 \bullet B(C_6F_5)_3$

9	-2.449999	-0.266838	2.628107
9	-0.913409	-2.623267	1.408209
9	-2.696200	-0.371689	-2.083516
9	0.316230	-0.721785	-2.733034
9	-1.343926	2.330774	1.390586
9	1.557978	-1.400346	1.493071
9	0.061756	3.448942	3.357275
9	-5.354837	-0.594155	-1.927628
9	-0.063924	-5.014086	0.548609
9	2.222062	2.170111	4.395244
9	-5.096988	-0.522274	2.758079
8	-0.695415	1.034707	-0.995400
8	1.463560	1.156322	-1.073692
9	2.928349	-0.265096	3.438933
9	1.067583	-5.243949	-1.914337
9	1.262672	-3.065753	-3.509852
9	-6.574609	-0.681596	0.491778
6	0.285635	1.702309	-1.344460
6	0.097792	2.991978	-1.999065
6	0.007375	0.391903	1.349778
6	-2.450153	-0.265926	0.262382
6	-0.305389	1.647286	1.877781
6	-3.252223	-0.376549	-0.874198

6	-0.311757	-1.553137	-0.593013
6	-0.417257	-2.710465	0.178313
6	0.208099	-1.736574	-1.869700
6	-3.118260	-0.331082	1.483345
6	1.123158	-0.221222	1.918426
6	0.410215	2.261136	2.900385
6	1.519551	1.609468	3.433317
6	1.870777	0.357258	2.945327
6	0.027389	-3.959304	-0.238623
6	-1.090316	3.671881	-1.679737
1	-1.768594	3.238693	-0.939844
6	0.984260	3.524029	-2.948975
1	1.895984	2.989534	-3.218591
6	-4.637020	-0.503859	-0.822436
6	0.679538	-2.966380	-2.325196
6	0.591760	-4.083596	-1.505312
6	-4.502878	-0.468278	1.579679
6	-5.264719	-0.553862	0.418822
6	-1.372357	4.886990	-2.286353
1	-2.285843	5.426816	-2.025484
6	0.676132	4.726758	-3.568791
1	1.355335	5.136828	-4.320169
6	-0.491749	5.411441	-3.231542
5	-0.842696	-0.169945	0.074032
8	2.549919	2.068011	-1.163466
6	3.695770	1.576116	-0.503180
8	4.466646	2.428446	-0.195503
6	3.848670	0.123605	-0.310425
6	4.571453	-0.273357	0.822313
6	3.410340	-0.835890	-1.233707

6	4.820344	-1.620373	1.050081
6	3.693146	-2.179170	-1.015131
6	4.384185	-2.571985	0.130227
1	2.862258	-0.539547	-2.132405
1	3.367817	-2.923263	-1.748856
1	5.357450	-1.928833	1.950555
1	4.914388	0.486315	1.530705
1	4.587380	-3.632347	0.304470
1	-0.718818	6.365316	-3.715998

$(p\text{-}BrC_6H_4COO)_2 \bullet B(C_6F_5)_3$

9	0.019964	3.159396	2.396348
9	-2.330376	2.549302	0.475808
9	1.267220	2.615317	-2.124297
9	-0.146934	-0.245472	-2.642411
9	2.104772	0.928961	2.082683
9	-2.424732	-0.118642	1.208066
9	1.912824	-0.308205	4.432106
9	2.155088	5.134944	-2.167739
9	-4.540096	2.481757	-1.031371
9	-0.427784	-1.466815	5.183556
9	0.900876	5.662256	2.324829
8	1.369787	0.420996	-0.507627
8	0.539497	-1.576578	-0.404820
9	-2.575304	-1.340837	3.536102
9	-4.579019	0.999339	-3.314034
9	-2.355229	-0.343216	-4.076838
9	1.974269	6.681900	0.055079
6	1.604721	-0.794324	-0.528824
6	2.968340	-1.281597	-0.681274

6	-0.150492	0.497905	1.521793
6	0.635741	2.751616	0.145683
6	0.924665	0.392634	2.407861
6	1.178108	3.327802	-1.004102
6	-1.141206	1.141064	-0.978795
6	-2.297330	1.853137	-0.655518
6	-1.191339	0.455485	-2.187442
6	0.549557	3.588427	1.256659
6	-1.327284	-0.111539	1.955091
6	0.859762	-0.247577	3.640419
6	-0.337707	-0.843479	4.027808
6	-1.437953	-0.765720	3.183224
6	-3.461859	1.826922	-1.414205
6	3.988405	-0.421662	-0.239098
1	3.718334	0.525318	0.235137
6	3.296752	-2.504856	-1.288913
1	2.514138	-3.172730	-1.651501
6	1.642876	4.639152	-1.055919
6	-2.333584	0.406260	-2.984760
6	-3.480075	1.083101	-2.591495
6	0.998013	4.908065	1.245577
6	1.547067	5.435492	0.081166
6	5.317273	-0.788445	-0.375223
1	6.114681	-0.135766	-0.012543
6	4.626182	-2.858875	-1.452182
1	4.893233	-3.799462	-1.939347
6	5.628956	-2.005063	-0.985396
5	0.089204	1.225973	0.078742
8	0.851239	-2.921930	-0.066667
6	-0.254000	-3.575958	0.521745

8	0.050003	-4.495252	1.213091
6	-1.613537	-3.119490	0.192325
6	-2.599788	-3.371511	1.156485
6	-1.975945	-2.558094	-1.040547
6	-3.919319	-3.012251	0.924819
6	-3.301618	-2.233937	-1.292174
6	-4.259591	-2.433443	-0.297721
1	-1.230860	-2.380620	-1.821172
1	-3.597583	-1.823501	-2.261608
1	-4.682448	-3.166625	1.691375
1	-2.312228	-3.827262	2.108396
35	7.429186	-2.504605	-1.183712
35	-6.030617	-1.882608	-0.613365

$(p\text{-}MeC_6H_4COO)_2 \bullet B(C_6F_5)_3$

9	-2.416440	-0.228198	2.651749
9	-0.837438	-2.565032	1.474054
9	-2.735750	-0.359853	-2.055633
9	0.239140	-0.743391	-2.748839
9	-1.380319	2.369524	1.364461
9	1.580372	-1.313894	1.517685
9	-0.000806	3.529748	3.324101
9	-5.387603	-0.617310	-1.855766
9	0.186423	-4.918168	0.699153
9	2.174063	2.294859	4.385911
9	-5.054876	-0.524219	2.825097
8	-0.700302	1.050197	-1.001068
8	1.462124	1.116661	-1.118641
9	2.922337	-0.138718	3.455434
9	1.261003	-5.176904	-1.779672

9	1.228254	-3.075385	-3.486037
9	-6.567182	-0.714087	0.583328
6	0.293542	1.694984	-1.367978
6	0.124525	2.986705	-2.013770
6	0.002627	0.452384	1.346379
6	-2.452045	-0.241412	0.285368
6	-0.331145	1.708507	1.859619
6	-3.271046	-0.366718	-0.837242
6	-0.310153	-1.527534	-0.567465
6	-0.351363	-2.663877	0.241116
6	0.177044	-1.733582	-1.854247
6	-3.100359	-0.309422	1.516918
6	1.127095	-0.134788	1.924251
6	0.370051	2.343772	2.879335
6	1.486873	1.715233	3.423930
6	1.861882	0.465511	2.947474
6	0.165099	-3.897201	-0.137682
6	-1.054675	3.683700	-1.695361
1	-1.740327	3.258847	-0.957461
6	1.015659	3.525651	-2.957032
1	1.925370	2.990181	-3.230805
6	-4.653207	-0.513027	-0.762386
6	0.680145	-2.959073	-2.286195
6	0.694167	-4.039946	-1.416200
6	-4.481012	-0.466608	1.636675
6	-5.260374	-0.567635	0.488708
6	-1.318905	4.905138	-2.291002
1	-2.225836	5.454427	-2.020246
6	0.720258	4.734747	-3.563720
1	1.411024	5.145058	-4.306945

6	-0.442635	5.449237	-3.239412
5	-0.845974	-0.134052	0.077849
8	2.571437	1.999849	-1.229485
6	3.717613	1.492199	-0.574502
8	4.498629	2.338269	-0.272652
6	3.850122	0.041468	-0.383292
6	4.579715	-0.377135	0.737298
6	3.378424	-0.914554	-1.294295
6	4.773445	-1.729855	0.979281
6	3.620067	-2.259894	-1.063631
6	4.288854	-2.694167	0.088517
1	2.832921	-0.610914	-2.192504
1	3.276070	-3.003701	-1.790708
1	5.302994	-2.048113	1.882670
1	4.969917	0.374493	1.429337
6	4.476373	-4.156913	0.332308
1	3.550771	-4.716946	0.118808
1	5.255585	-4.570684	-0.330482
1	4.775851	-4.364731	1.369683
6	-0.751085	6.745347	-3.912847
1	0.163743	7.309315	-4.149427
1	-1.275823	6.568015	-4.867769
1	-1.405036	7.379678	-3.296669

$(PhCOO)_2 \cdot 2B(C_6F_5)_3$

9	5.795465	2.016776	-0.191495
9	5.543459	-0.597288	-1.778679
9	5.627793	-1.817657	2.554446
9	3.025103	-3.181148	1.267788
9	3.481244	2.168886	1.806139

9	2.763062	-0.356366	-2.129139
9	2.006956	4.135053	0.789861
9	8.028168	-1.196949	3.547624
9	5.839222	-2.751170	-3.337896
9	0.902294	3.872457	-1.693457
9	8.193012	2.604881	0.801244
8	3.304163	-0.617370	2.006282
8	1.384790	-1.114123	1.165236
9	1.308755	1.616049	-3.103429
9	4.644492	-5.097446	-2.651616
9	3.222642	-5.253006	-0.349509
9	9.332366	1.017248	2.675199
6	2.099386	-0.728670	2.238404
6	1.547620	-0.437229	3.554760
6	3.234714	0.806664	-0.108130
6	5.577640	0.090808	1.165138
6	2.974322	1.993314	0.584112
6	6.217593	-0.709336	2.113514
6	4.253966	-1.762185	-0.198566
6	4.998228	-1.741074	-1.379043
6	3.723014	-3.001753	0.141725
6	6.293999	1.205776	0.733081
6	2.637559	0.725438	-1.367089
6	2.207294	3.041449	0.081765
6	1.643728	2.914599	-1.184667
6	1.865389	1.752138	-1.910191
6	5.152670	-2.840444	-2.215657
6	2.370076	0.359699	4.376996
1	3.329855	0.710557	3.990470
6	0.309122	-0.895375	4.045801

1	-0.342631	-1.526843	3.444545
6	7.470687	-0.413324	2.642659
6	3.835589	-4.126108	-0.675040
6	4.554699	-4.047032	-1.859924
6	7.553357	1.534155	1.232347
6	8.143127	0.718918	2.193298
6	1.948756	0.712730	5.648856
1	2.583617	1.343612	6.275369
6	-0.097254	-0.539652	5.322841
1	-1.066483	-0.885505	5.689981
6	0.714041	0.267011	6.120161
5	4.125183	-0.359598	0.607635
8	-0.002023	-0.960822	1.354208
6	-0.685433	-0.897489	0.180553
8	-1.789096	-0.429756	0.374546
6	-0.141336	-1.395714	-1.070594
6	-0.470455	-0.703921	-2.246780
6	0.565251	-2.609415	-1.127017
6	-0.081883	-1.220359	-3.474831
6	0.917338	-3.130834	-2.364279
6	0.598388	-2.436379	-3.532507
5	-3.317923	-0.069739	-0.081388
6	-4.150678	-0.667955	1.180006
6	-3.703328	-0.504795	2.493731
6	-5.354244	-1.359004	1.038108
6	-4.376789	-1.025491	3.596019
6	-6.065087	-1.880453	2.117399
6	-5.569838	-1.713798	3.406833
6	-3.305214	1.551822	-0.073467
6	-4.523920	2.217783	0.057714

6	-2.179820	2.370806	-0.102142
6	-4.631975	3.598007	0.192175
6	-2.235223	3.754320	0.057792
6	-3.472923	4.371388	0.199215
6	-3.537807	-0.820153	-1.493274
6	-3.256353	-2.182425	-1.599642
6	-3.951837	-0.198399	-2.669460
6	-3.335672	-2.896271	-2.788620
6	-4.060232	-0.878786	-3.883834
6	-3.750828	-2.233785	-3.942021
9	-0.949158	1.865089	-0.285133
9	-1.130440	4.474138	0.072055
9	-3.549425	5.678001	0.338745
9	-5.809081	4.178688	0.314168
9	-5.650834	1.514525	0.042277
1	0.804880	-3.160310	-0.212540
1	1.442012	-4.089502	-2.417652
1	-0.306777	-0.666881	-4.390091
1	-0.986823	0.258432	-2.183034
9	-7.199226	-2.526856	1.930606
9	-6.223107	-2.204722	4.439370
9	-3.892997	-0.867016	4.818834
9	-2.577109	0.158028	2.760815
9	-5.884686	-1.550030	-0.162420
9	-2.848176	-2.855437	-0.520880
9	-3.026995	-4.178013	-2.836855
9	-3.844022	-2.886084	-5.081697
9	-4.451983	-0.249970	-4.974718
9	-4.248787	1.093775	-2.690167
1	0.378462	0.552225	7.121155

1	0.890629	-2.848843	-4.502027

$(p\text{-}BrC_6H_4COO)_2 \cdot 2B(C_6F_5)_3$

9	5.758111	2.018534	-0.194140
9	5.508652	-0.587143	-1.792226
9	5.617843	-1.824202	2.541969
9	3.024057	-3.201832	1.256096
9	3.450774	2.151359	1.818026
9	2.733793	-0.353276	-2.131296
9	1.999843	4.134455	0.798634
9	8.017829	-1.194536	3.529200
9	5.806328	-2.729849	-3.365020
9	0.917001	3.893856	-1.694910
9	8.156053	2.614855	0.791997
8	3.288885	-0.636161	2.006677
8	1.366740	-1.157694	1.186184
9	1.310053	1.638508	-3.109971
9	4.631919	-5.088359	-2.681922
9	3.232713	-5.266219	-0.367951
9	9.308961	1.028225	2.658307
6	2.086322	-0.753115	2.248722
6	1.544324	-0.451687	3.564371
6	3.205634	0.798467	-0.103196
6	5.554185	0.087124	1.157182
6	2.949283	1.984258	0.592462
6	6.201131	-0.712145	2.101573
6	4.235091	-1.767130	-0.210438
6	4.971701	-1.735949	-1.395804
6	3.715176	-3.012192	0.127279
6	6.263867	1.206812	0.725963

6	2.614933	0.727636	-1.365758
6	2.196943	3.042084	0.088016
6	1.643557	2.926462	-1.183880
6	1.859192	1.764669	-1.911935
6	5.127311	-2.829693	-2.239802
6	2.379049	0.336795	4.383007
1	3.342859	0.674675	3.994516
6	0.302886	-0.889894	4.067010
1	-0.361322	-1.517172	3.475199
6	7.454338	-0.411421	2.627734
6	3.832062	-4.132162	-0.694912
6	4.539226	-4.042092	-1.886437
6	7.523230	1.539912	1.222092
6	8.120011	0.725136	2.179168
6	1.976691	0.701561	5.655015
1	2.617631	1.324600	6.282911
6	-0.098315	-0.528799	5.342001
1	-1.069476	-0.856228	5.721237
6	0.735077	0.269841	6.128929
5	4.102130	-0.369276	0.603339
8	-0.021657	-1.008353	1.374691
6	-0.692617	-0.906424	0.193460
8	-1.780973	-0.401056	0.378588
6	-0.141336	-1.410506	-1.049419
6	-0.431572	-0.714984	-2.234032
6	0.552107	-2.632714	-1.096205
6	-0.013736	-1.222210	-3.454183
6	0.928994	-3.160897	-2.319845
6	0.651391	-2.449959	-3.491201
5	-3.313377	-0.049121	-0.086316

6	-4.145790	-0.654177	1.172033
6	-3.702459	-0.494777	2.487568
6	-5.343962	-1.353809	1.024512
6	-4.369961	-1.032014	3.585398
6	-6.049835	-1.890656	2.099480
6	-5.556205	-1.730408	3.390479
6	-3.306637	1.570967	-0.081824
6	-4.525370	2.235198	0.055929
6	-2.182498	2.390811	-0.120749
6	-4.633684	3.615512	0.190056
6	-2.237753	3.774092	0.039404
6	-3.475213	4.389983	0.189017
6	-3.522150	-0.805283	-1.496061
6	-3.233001	-2.166257	-1.598293
6	-3.950067	-0.191868	-2.671703
6	-3.321326	-2.888001	-2.781827
6	-4.064837	-0.879547	-3.881469
6	-3.750796	-2.233876	-3.935057
9	-0.953548	1.884807	-0.314316
9	-1.133084	4.494131	0.045386
9	-3.552119	5.696410	0.328381
9	-5.810381	4.195172	0.318715
9	-5.651170	1.530272	0.047706
1	0.768733	-3.190694	-0.180441
1	1.440387	-4.126376	-2.374239
1	-0.193642	-0.665812	-4.377311
1	-0.942614	0.251388	-2.185796
9	-7.177668	-2.546088	1.907142
9	-6.204136	-2.237289	4.418238
9	-3.886239	-0.879373	4.808848

9	-2.584420	0.179268	2.761443
9	-5.872988	-1.539137	-0.177553
9	-2.810544	-2.830844	-0.518667
9	-3.008807	-4.168742	-2.824694
9	-3.853394	-2.892790	-5.069193
9	-4.470268	-0.258943	-4.971614
9	-4.258963	1.097189	-2.694434
35	0.179499	0.770967	7.848578
35	1.210998	-3.153394	-5.136902

$(p\text{-}MeC_6H_4COO)_2 \cdot 2B(C_6F_5)_3$

9	5.885131	1.875521	-0.140842
9	5.252084	-0.526310	-1.882980
9	5.615132	-2.063133	2.442537
9	3.011675	-3.219071	1.283802
9	3.774716	2.069267	2.077613
9	2.525711	-0.087750	-1.943237
9	2.360701	4.198072	1.348369
9	8.123285	-1.667020	3.285285
9	5.251361	-2.580013	-3.604376
9	1.023772	4.212028	-1.017466
9	8.386899	2.233643	0.689157
8	3.314603	-0.686768	2.077155
8	1.388272	-1.144357	1.218659
9	1.145404	2.049340	-2.639394
9	4.097075	-4.935835	-2.902097
9	2.982685	-5.207546	-0.451153
9	9.528550	0.480822	2.408791
6	2.100756	-0.765345	2.297835
6	1.535036	-0.446788	3.593584

6	3.255779	0.878943	0.101501
6	5.613929	-0.088251	1.151834
6	3.148334	2.021311	0.900251
6	6.256391	-0.979891	2.012028
6	4.099476	-1.746418	-0.238012
6	4.708753	-1.673407	-1.491357
6	3.589087	-2.996014	0.100789
6	6.383379	0.986403	0.709356
6	2.544061	0.937826	-1.096914
6	2.417315	3.151584	0.548091
6	1.728219	3.163218	-0.661155
6	1.801038	2.051412	-1.490673
6	4.727675	-2.724674	-2.401424
6	2.351676	0.341287	4.431641
1	3.329178	0.667233	4.069237
6	0.275000	-0.867484	4.066358
1	-0.373656	-1.502484	3.464054
6	7.563867	-0.803953	2.456859
6	3.593672	-4.079074	-0.776398
6	4.157618	-3.940589	-2.036333
6	7.698143	1.194515	1.123112
6	8.288839	0.294240	2.004094
6	1.904712	0.721997	5.683078
1	2.541994	1.345916	6.317052
6	-0.151779	-0.482960	5.324300
1	-1.135902	-0.807566	5.674062
6	0.642533	0.326618	6.149593
5	4.099655	-0.400337	0.669971
8	0.005852	-0.904922	1.367740
6	-0.629697	-0.761730	0.170974

8	-1.687211	-0.174817	0.333363
6	-0.092290	-1.299542	-1.056675
6	-0.358448	-0.607053	-2.247907
6	0.558336	-2.547854	-1.097723
6	0.058108	-1.135040	-3.459526
6	0.917578	-3.082019	-2.320279
6	0.696862	-2.379814	-3.517528
5	-3.255386	-0.010486	-0.098717
6	-3.999867	-0.643777	1.204430
6	-3.548162	-0.398098	2.504145
6	-5.136925	-1.447818	1.109998
6	-4.148436	-0.950842	3.633528
6	-5.774520	-2.003912	2.217367
6	-5.270849	-1.758242	3.490423
6	-3.446614	1.593630	-0.196680
6	-4.732580	2.119542	-0.077073
6	-2.434850	2.527870	-0.404248
6	-5.009536	3.481439	-0.114030
6	-2.664274	3.902835	-0.437633
6	-3.961184	4.381219	-0.288004
6	-3.422605	-0.848733	-1.472724
6	-3.024241	-2.185461	-1.518131
6	-3.891288	-0.324128	-2.676225
6	-3.027858	-2.955875	-2.673264
6	-3.934657	-1.067629	-3.856890
6	-3.498126	-2.387781	-3.855045
9	-1.164870	2.142642	-0.597543
9	-1.669807	4.749326	-0.617926
9	-4.198676	5.676182	-0.320645
9	-6.244981	3.926591	0.003986

9	-5.768442	1.294517	0.039231
1	0.749858	-3.112438	-0.179755
1	1.389907	-4.070015	-2.359879
1	-0.108839	-0.570731	-4.381956
1	-0.854232	0.366805	-2.204589
9	-6.846239	-2.759098	2.071467
9	-5.851513	-2.281750	4.550208
9	-3.662619	-0.709886	4.843600
9	-2.496642	0.387495	2.733699
9	-5.674895	-1.718285	-0.071756
9	-2.556149	-2.765756	-0.407844
9	-2.587562	-4.200656	-2.669372
9	-3.517925	-3.094183	-4.965839
9	-4.380703	-0.529841	-4.975344
9	-4.310956	0.930473	-2.763161
6	0.143743	0.780205	7.479586
1	-0.364180	1.755634	7.382211
1	-0.588299	0.076964	7.902672
1	0.964516	0.915674	8.199497
6	1.148972	-2.967429	-4.811816
1	2.216102	-3.242034	-4.763863
1	0.593686	-3.894042	-5.034731
1	1.007321	-2.273230	-5.651709

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