Electronic Supporting Information

Electron-deficient cyclopropenium cations as Lewis acids in FLP chemistry

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Table S1. TPSS-D3/def2-TZVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in CH_2Cl_2 solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95-D3); the total PW6B95-D3 free energies G_P; the relative electronic energies (ΔE_T and ΔE_P) and Gibbs energies (ΔG_T and ΔG_P) at the TPSS-D3 and PW6B95-D3 levels. (group Ph = C_6H_5; tBu = CMe_3; To = *o*-$C_6H_5CH_3$) 88

Table S2. TPSS-D3/def2-TZVP + COSMO optimized Cartesian coordinates (in Å) in CH_2Cl_2 solution. Each structure is labeled by a specific name (See Table S1), followed by the number of atoms, the total energy (in hartrees), and the detailed atomic coordinates (in double-column text list). 91

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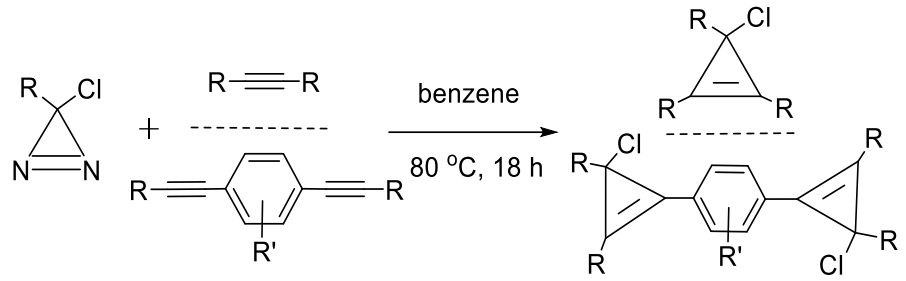
Experimental

General information for synthesis

Experiments were carried under inert conditions using standard Schlenk techniques or a glove box as appropriate. Dichloromethane (DCM, CH_2Cl_2), toluene ($PhCH_3$) and *n*-hexanes (C_6H_{14}) were dispensed from an MBRAUN Solvent Purification System, deoxygenated by bubbling nitrogen for 20 min, and stored over 3 Å molecular sieves prior to use. Chloroform-d ($CDCl_3$) and Acetonitrile-d_3 (CD_3CN) solvents were used as received without any purification and those were stored over 4 Å molecular sieves prior to use. Vials and stir bar for reactions were oven-dried overnight before experiments. ^{1}H (400 MHz), ^{19}F (377 MHz), ^{31}P (162 MHz), ^{11}B (128 MHz) and $^{13}C\{^{1}H\}$ (101 MHz) NMR spectra were run at 298 K on Bruker 400 spectrometer. The chemical shifts (δ, ppm) for ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra are given relative to solvent signals whereas an external reference standards used for ^{19}F ($CFCl_3$), 31P (85% H_3PO_4) and ^{11}B ($BF_3{\cdot}OEt_2$) NMR spectra. These NMR data are given as: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz) and integration. The single-crystal *X*-ray data were collected on a Bruker Kappa Apex II diffractometer which was equipped with rotation anode using graphite-monochromated MoKα radiation (λ = 0.71073 Å) at 150 K. Structures were solved and refined using Full-matrix least-squares based on F^2 with a suite of programs SHELXS and SHELXL[1] compiled in OLEX2.[2] High-resolution mass spectra (HRMS) were obtained on an AccuTOF Plus 4G (DART), Agilent 6538 UHD (ESI) or MALDI-TOF at AIMS Mass Spectrometry Laboratory whilst elemental (CHN) alaysis was performed on Thermo Scientific Flash 2000 CHNS Analyzer at ANALEST Facility, University of Toronto. The cyclic voltammetry (CV) was performed with a three-electrode system, glassy carbon as working electrode whilst platinum wire as an auxiliary electrode and Ag/AgCl as a reference electrode. The experiments were performed with a 10^{-3} M solution of sample in CH_3CN/DCM (1:1) containing 0.1 M $[(n\text{-}Bu)_4N]PF_6$ as supporting electrolyte with a scan rate 0.1 V/s. The reagents $B(C_6F_5)_3$[3], $Et_3SiB(C_6F_5)_4$[4] and aryl(chloro)cyclopropenes[5] were prepared following

literature protocols. Notably, a general synthesis for aryl(chloro)cyclopropenes is added in the later section. All other reagents were purchased commercially and used as received.

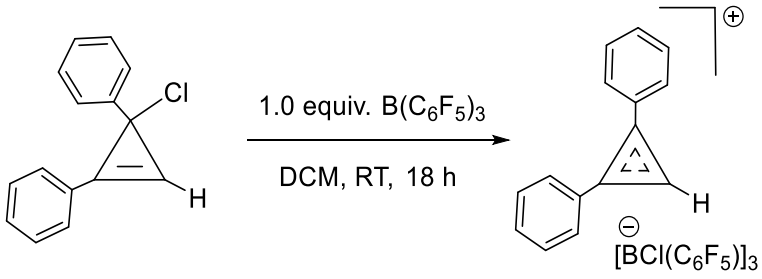
General synthesis for aryl(chloro)cyclopropenes[5]



Into an 20 mL vial equipped with a stir bar, a suitable aryl(chloro)diazirine[6] (0.50 mmol, 1.0 equiv.) was taken in benzene (5.0 mL). A solution of an appropriate alkyne (0.50 mmol, 1.0 equiv.) in benzene (5.0 mL) was transferred to the vial. The reaction mixture was allowed to stir at 80 °C for 18 h. After removal of all volatiles, the residue was treated with mimimum *n*-hexanes and dried again. The resultant materials were used directly without any further purification. Notably, the synthesis of aryl(chloro)cyclopropenes from pentafluorophenyl(chloro)diazirine, $[(C_6F_5)C(N_2)Cl]$[7] with alkynes were performed in hexafluorobenzene (C_6F_6) instead of benzene and the resultant crude reaction mixtures were used directly for halide abstraction reactions.

Synthetic procedures and characterization data

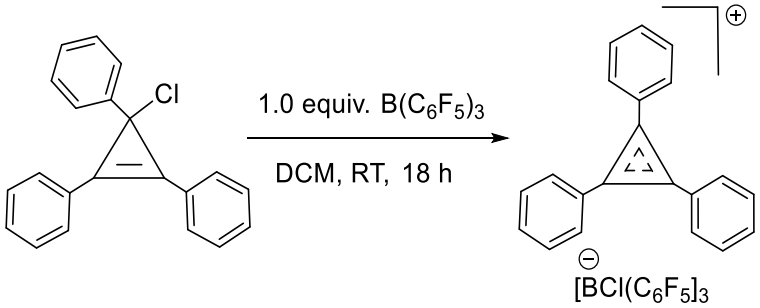
Synthesis 1



Into a 4 mL vial equipped with a stir bar, $B(C_6F_5)_3$ (51.1 mg, 0.10 mmol, 1.0 equiv.) was taken in DCM (0.5 mL). A solution of 1,2-bis(phenyl)-(1-chloro)-2-cyclopropene (22.7 mg, 0.10 mmol, 1.0 equiv.) in DCM (0.5 mL) was transferred to the vial. The reaction mixture was allowed to stir at RT for 18 h. After removal of all volatiles, the residue was washed with *n*-hexane (3 x 3 mL) and followed by drying afforded compound **1** (56.9 mg, 77%). *X*-ray quality crystals were grown with a mixture of solvent of DCM:*n*-hexane (1:5) and stored at -

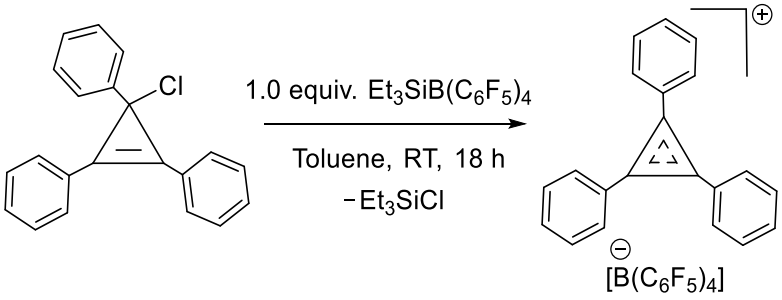
30 °C for a week. **1**: $C_{33}H_{11}BClF_{15}$ requires: C 53.7, H 1.50. Found: C 53.6, H 1.42%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 10.69 (br s, 1 H, $(Ph_2C)_2CH$), 8.34 (dt, *J* = 8.4, 1.4 Hz, 4 H, $(Ph_2C)_2CH$), 8.04 (tt, *J* = 7.5, 1.6 Hz, 2 H, $(Ph_2C)_2CH$), 7.94 - 7.70 (m, 4 H, $(Ph_2C)_2CH$); ^{19}F NMR (377 MHz, $CDCl_3$): δ_F -132.2 (m, 6 F, *o*-C_6F_5 of -$BCl(C_6F_5)_3$), -159.9 (m, 3 F, *p*-C_6F_5 of -$BCl(C_6F_5)_3$), -165.4 (m, 6 F, *m*-C_6F_5 of -$BCl(C_6F_5)_3$); ^{11}B NMR (128 MHz, $CDCl_3$): δ_B -5.9 (br s, 1 B, -$BCl(C_6F_5)_3$); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 160.5 (br m, -C_6F_5), 149.2 (br s, -C_6F_5), 146.8 (br m, -C_6F_5), 140.4 (br m, -C_6F_5), 140.2 (s, C_{Ar} of Ph), 138.0 (br m, -C_6F_5), 136.3 (s, C_{Ar} of Ph), 135.6 (br m, -C_6F_5), 131.0 (s, C_{Ar} of Ph), 127.8 (*C*=*C* of Ph_2C_3), 118.4 (s, C_{Ar} of Ph); HRMS (ESI, Positive) m/z: 191.0862 for [M^+] (calcd.: 191.0855 for $C_{15}H_{11}^+$).

Synthesis 2a



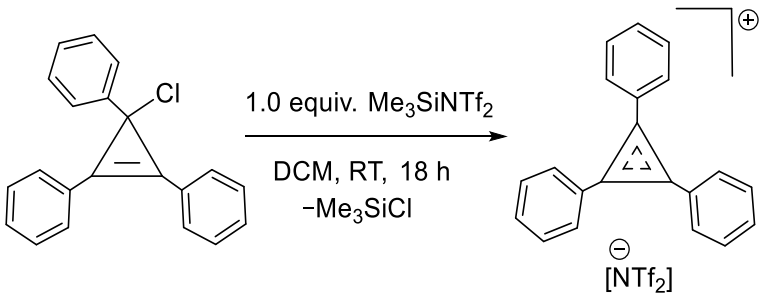
2a was prepared by following the protocol for **1** whereas 1,2,3-tris(phenyl)-(1-chloro)-2-cyclopropene (30.2 mg, 0.10 mmol, 1.0 equiv.) was used. After removal of all volatiles, the residue was washed with *n*-hexane (3 x 3 mL) and followed by crystallization with a mixture of solvent of DCM:*n*-hexane (1:5) and stored at -30 °C for three days afforded compound **2a** (71 mg, 87%). **2a**: ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.56 - 8.34 (m, 6 H, Ar*H*), 8.01 (tt, *J* = 7.1, 1.7 Hz, 3 H, Ar*H*), 7.92 - 7.78 (m, 6 H, Ar*H*); ^{19}F NMR (377 MHz, $CDCl_3$): δ_F -132.1 (m, 6 F, *o*-C_6F_5 of -$BCl(C_6F_5)_3$), -161.7 (m, 3 F, *p*-C_6F_5 of -$BCl(C_6F_5)_3$), -166.5 (m, 6 F, *m*-C_6F_5 of -$BCl(C_6F_5)_3$); ^{11}B NMR (128 MHz, $CDCl_3$): δ_B -7.2 (br s, 1 B, -$BCl(C_6F_5)_3$); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 154.9 (s, $Ph_3C_3^+$), 149.1 (br m, -C_6F_5), 146.8 (br m, -C_6F_5), 141.4 (br m, -C_6F_5), 139.8 (br m, -C_6F_5), 138.9 (s, C_{Ar} of Ph), 135.3 (s, C_{Ar} of Ph), 130.9 (s, C_{Ar} of Ph), 119.6 (s, C_{Ar} of Ph).

Synthesis 2b



2b was prepared by following the protocol for **1** whereas 1,2,3-(trisphenyl)-(1-chloro)-2-cyclopropene (30.2 mg, 0.10 mmol, 1.0 equiv.), $Et_3Si[B(C_6F_5)_4]$ (79.0 mg, 0.10 mmol, 1.0 equiv.) were used and the reaction was carried out in toluene (2.0 mL). After stirring at RT for 18 h, the toluene layer was pipetted out. The oily residue was washed with *n*-hexane (3 x 3 mL) followed by crystallization with a mixture of solvent of DCM:*n*-hexane (1:5) and stored at -30 °C for three days afforded compound **2b** (86 mg, 91%). **2b**: $C_{45}H_{15}BF_{20}$ requires: C 57.1, H 1.60. Found: C 57.5, H 1.38%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.50 - 8.33 (m, 6 H, Ar*H*), 8.03 (tt, *J* = 7.4, 1.8 Hz, 3 H, Ar*H*), 7.93 - 7.80 (m, 6 H, Ar*H*); ^{19}F NMR (377 MHz, $CDCl_3$): δ_F -132.5 (m, 6 F, *o*-C_6F_5 of -$BArF_{20}$), -162.8 (m, 3 F, *p*-C_6F_5 of -$BArF_{20}$), -166.7 (m, 6 F, *m*-C_6F_5 of -$BArF_{20}$); ^{11}B NMR (128 MHz, $CDCl_3$): δ_B -16.8 (br s, 1 B, -$BArF_{20}$); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 155.4 (s, $Ph_3C_3^+$), 149.7 (br m, -C_6F_5), 147.3 (br m, -C_6F_5), 139.8 (s, C_{Ar} of Ph), 139.6 (br m, -C_6F_5), 137.8 (br m, -C_6F_5), 137.3 (br s, -C_6F_5), 135.6 (s, C_{Ar} of Ph), 135.4 (br m, -C_6F_5), 131.5 (s, C_{Ar} of Ph), 119.6 (s, C_{Ar} of Ph); HRMS (ESI, Positive) m/z: 267.1176 for [M^+] (calcd.: 267.1168 for $C_{21}H_{15}^+$).

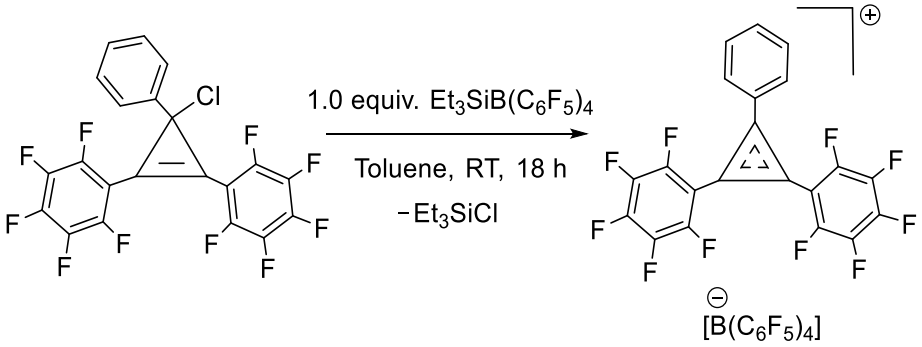
Synthesis 2c



2c was prepared by following the protocol for **1** whereas 1,2,3-(trisphenyl)-(1-chloro)-2-cyclopropene (30.2 mg, 0.10 mmol, 1.0 equiv.), Me_3SiNTf_2 (35.3 mg, 0.10 mmol, 1.0 equiv.)

were used. After removal of all volatiles, the residue was washed with *n*-hexane (3 x 3 mL) and followed by crystallization with a mixture of solvent of DCM:*n*-hexane (1:5) and stored at -30 °C for three days afforded compound **2c** (43 mg, 76%). **2c**: ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 8.56 - 8.42 (m, 6 H, Ar*H*), 8.02 (tt, *J* = 7.4, 1.6 Hz, 3 H, Ar*H*), 7.96 - 7.83 (m, 6 H, Ar*H*); ^{19}F NMR (377 MHz, $CDCl_3$): δ_F -79.1 (s, 6 F, NTf_2); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 155.7 (s, $Ph_3C_3^+$), 139.3 (s, C_{Ar} of Ph), 135.9 (s, C_{Ar} of Ph), 131.2 (s, C_{Ar} of Ph), 120.1 (q, *J* = 322 Hz, CF_3 of NTf_2), 120.0 (s, C_{Ar} of Ph).

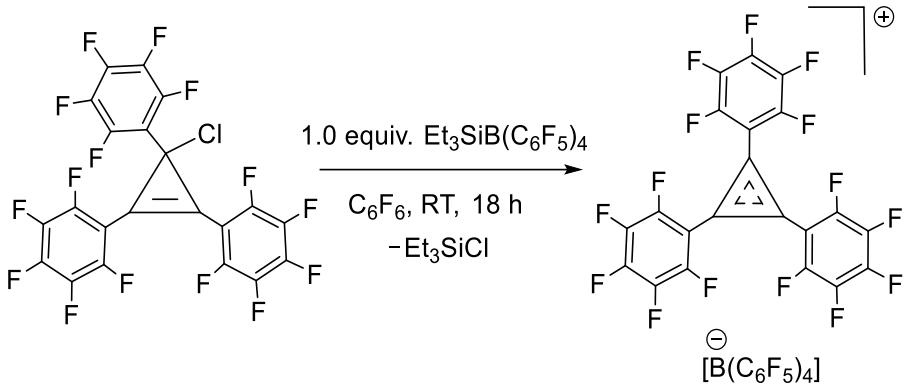
Synthesis 3



3 was prepared by following the protocol for **1** whereas 1-(phenyl)-2,3-bis(pentafluorophenyl)-(1-chloro)-2-cyclopropene (48.3 mg, 0.10 mmol, 1.0 equiv.), $Et_3Si[B(C_6F_5)_4]$ (79.0 mg, 0.10 mmol, 1.0 equiv.) were taken and the reaction was in toluene (2.0 mL). After stirring at RT for 18 h, the toluene layer was pipetted out. The residue was washed with *n*-hexane (3 x 3 mL) followed by drying afforded brownish-yellow powder compound **3** (103 mg, 91%). *X*-ray quality crystals were grown with the mixture of solvents using DCM:CH_3CN:*n*-hexanes (1:1:5) and -30 °C for seven days. **3**: $C_{45}H_5BF_{30}$ requires: C 48.0, H 0.45. Found: C 51.2, H 1.01%. ^{1}H NMR (400 MHz, CD_3CN): δ_H 8.51 (d, *J* = 7.6, Hz, 2 H, Ar-*H*), 8.15 (tt, *J* = 7.5, 1.3 Hz, 1 H, Ar-*H*), 7.99 - 7.88 (m, 2 H, Ar-*H*); ^{19}F NMR (377 MHz, CD_3CN): δ_F -128.4 (m, 4 F, *o*-C_6F_5 of -$C_3(C_6F_5)_2Ph$), -133.8 (m, 8 F, *o*-C_6F_5 of -$B(C_6F_5)_4$), -134.9 (m, 2 F, *p*-C_6F_5 of -$C_3(C_6F_5)_2Ph$), -159.0 (m, 4 F, *m*-C_6F_5 of -$C_3(C_6F_5)_2Ph$), -164.0 (m, 4 F, *p*-C_6F_5 of -$B(C_6F_5)_4$), -168.4 (m, 8 F, *m*-C_6F_5 of -$B(C_6F_5)_4$); ^{11}B NMR (128 MHz, CD_3CN): δ_B -16.7 (br s, 2 B, -*B*$(C_6F_5)_4$); ^{13}C NMR (101 MHz, CD_3CN): δ_C 158.4 (s, $((C_6F_5)_2PhC_3)^+$), 150.2 (br m, -C_6F_5), 147.8 (br m, -C_6F_5), 147.5 (br m, -C_6F_5), 142.0 (s, C_{Ar} of

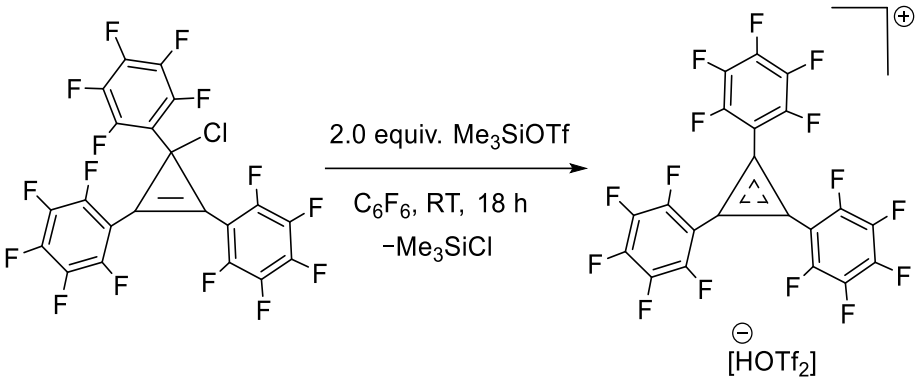
Ph), 141.0 (br m, -C_6F_5), 140.5 (br m, -C_6F_5), 138.6 (br m, -C_6F_5), 138.2 (s, C_{Ar} of Ph),138.1 (br m, -C_6F_5), 136.1 (br m, -C_6F_5), 131.9 (C_{Ar} of Ph), 119.3 (C_{Ar} of Ph); HRMS (ESI, Positive) m/z: 447.0236 for [M^+] (calcd.: 447.0226 for $C_{21}H_5F_{10}^+$).

Synthesis 4a



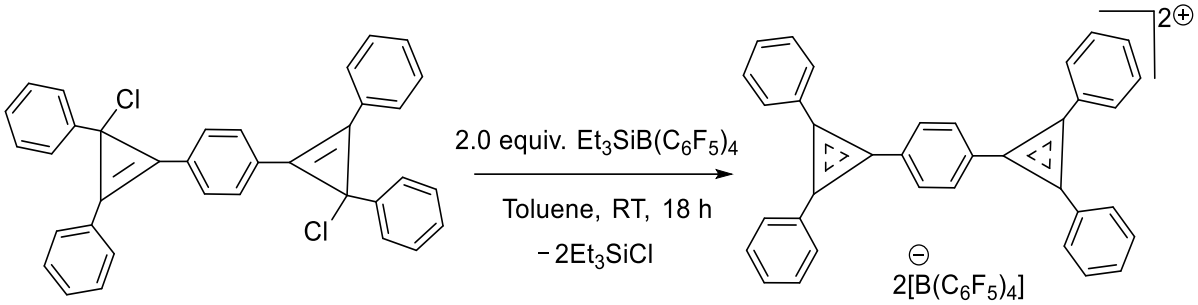
4a was prepared by following the protocol for **1** whereas 1,2,3-(trispentafluorophenyl)-(1-chloro)-2-cyclopropene (57.3 mg, 0.10 mmol, 1.0 equiv.), $Et_3Si[B(C_6F_5)_4]$ (79.0 mg, 0.10 mmol, 1.0 equiv.) were taken and the reaction was in C_6F_6 (2.0 mL). After stirring at RT for 18 h, the C_6F_6 layer was pipetted out. The residue was washed with *n*-hexane (3 x 3 mL) followed by drying afforded compound **4a** (106 mg, 87%). *X*-ray quality crystals were grown with the mixture of solvents using DCM:CH_3CN:*n*-hexanes (1:1:5) and left at -30 °C for a week. **4a**: $C_{45}BF_{35}$ requires: C 44.4. Found: C 44.0%. ^{19}F NMR (377 MHz, CD_3CN): δ_F -126.8 (m, 4 F, *o*-C_6F_5 of -$C_3(C_6F_5)_3$), -128.2 (m, 2 F, *o*-C_6F_5 of -$C_3(C_6F_5)_3$), -133.3 (m, 8 F, *o*-C_6F_5 of -$B(C_6F_5)_4$), -139.4 (m, 2 F, *p*-C_6F_5 of -$C_3(C_6F_5)_3$), -149.5 (m, 1 F, *p*-C_6F_5 of -$C_3(C_6F_5)_3$), -155.8 (m, 4 F, *m*-C_6F_5 of -$C_3(C_6F_5)_3$), -161.1 (m, 2 F, *m*-C_6F_5 of -$C_3(C_6F_5)_3$), -163.8 (m, 4 F, *p*-C_6F_5 of -$B(C_6F_5)_4$), -167.8 (m, 8 F, *m*-C_6F_5 of -$B(C_6F_5)_4$); ^{11}B NMR (128 MHz, CD_3CN): δ_B -16.7 (br s, 2 B, -$B(C_6F_5)_4$); ^{13}C NMR (101 MHz, CD_3CN): δ_C Not resolved C for $((C_6F_5)_3C_3)^+$, 149.0 (br m, -C_6F_5), 148.3 (br m, -C_6F_5), 146.8 (br m, -C_6F_5), 140.0 (br m, -C_6F_5), 139.2 (br m, -C_6F_5), 137.3 (br m, -C_6F_5), 136.8 (br m, -C_6F_5),134.8 (br m, -C_6F_5). HRMS (ESI, Positive) m/z: 536.9769 (M^+) (calcd.: 536.9755 for $C_{21}F_{15}^+$).

Synthesis 4b



4b (67 mg, 76%) was prepared by following the protocol for **4a** whereas Me_3SiOTf (44.4 mg, 0.2 mmol, 2 equiv.) was employed. X-ray suitable crystals were grown with the mixture of solvents using DCM:CH_3CN:*n*-hexanes (1:1:5) and left at -30 °C for a week. This batch of reaction was meant to be for better quality *X*-ray crystals, hence partial characterization data included here. **4b**: ^{1}H NMR (400 MHz, CD_3CN): δ_H 7.32 (br s, 1 H, [*H*OTf_2]$^-$); ^{19}F NMR (377 MHz, CD_3CN): δ_F -79.5 (m, 6 F, -C*F*$_3$ of [*H*OTf_2]$^-$), -138.2 (m, 4 F, *o*-C_6F_5 of -$C_3(C_6F_5)_3$), -143.3 (m, 2 F, *o*-C_6F_5 of $C_3(C_6F_5)_3^+$), -151.5 (m, 2 F, *p*-C_6F_5 of $C_3(C_6F_5)_3^+$), -157.7 (m, 1 F, *p*-C_6F_5 of $C_3(C_6F_5)_3^+$), -163.2 (m, 4 F, *m*-C_6F_5 of -$C_3(C_6F_5)_3$), -164.7 (m, 2 F, *m*-C_6F_5 of -$C_3(C_6F_5)_3$).

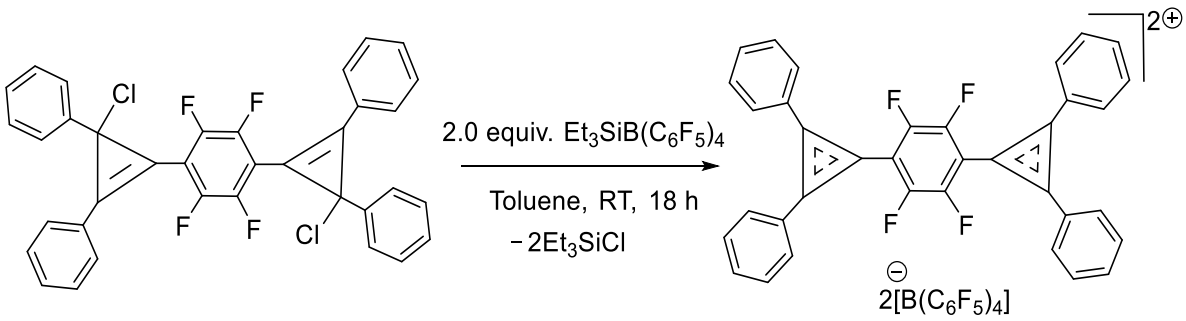
Synthesis 5



5 was prepared by following the protocol for **1** whereas 1,4-bis(3-chloro-2,3-diphenyl-1-cyclopropene)-benzene (52.8 mg, 0.10 mmol, 1.0 equiv.), $Et_3Si[B(C_6F_5)_4]$ (158.0 mg, 0.20 mmol, 2.0 equiv.) were employed in toluene (4.0 mL). After stirring at RT for 18 h, the toluene layer was pipetted out. The residue was washed with *n*-hexane (3 x 3 mL) followed by drying afforded yellow powder compound **5** (158 mg, 87%). *X*-ray quality crystals were grown with the mixture of solvents using DCM:CH_3CN:*n*-hexanes (1:1:5) at RT for a week. **5**:

^{1}H NMR (400 MHz, CD_3CN): δ_H 8.87 (s, 4 H, Ar-*H*), 8.63 (dt, *J* = 7.7, 1.5 Hz, 8 H, Ar-*H*), 8.12 (tt, *J* = 7.6, 1.7 Hz, 4 H, Ar-*H*), 8.02 - 7.87 (m, 8 H, Ar-*H*); ^{19}F NMR (377 MHz, CD_3CN): δ_F -133.7 (m, 16 F, *o*-C_6F_5 of -$B(C_6F_5)_4$), -163.8 (m, 8 F, *p*-C_6F_5 of -$B(C_6F_5)_4$), -168.4 (m, 16 F, *m*-C_6F_5 of -$B(C_6F_5)_4$); ^{11}B NMR (128 MHz, CD_3CN): δ_B -16.7 (br s, 2 B, -*B*$(C_6F_5)_4$); ^{13}C NMR (101 MHz, CD_3CN): δ_C Not resolved C for $(Ar_3C_3)^+$, 150.3 (br m, -C_6F_5), 147.9 (br m, -C_6F_5), 140.5 (br m, -C_6F_5), 140.2 (s, C_{Ar} of Ph), 138.6 (br m, -C_6F_5), 137.3 (s, C_{Ar} of Ph), 136.7 (s, C_{Ar} of Ph), 131.6 (s, C_{Ar} of Ph), 130.0 (s, C_{Ar} of Ph), 129.2 (s, C_{Ar} of Ph), 126.3 (s, C_{Ar} of Ph), 121.0 (C_{Ar} of Ph). Efforts to obtain EA or HRMS ddata for this highly Lewis acidic dication were unnssccessful. Nonetheless, full characterization of subsequent reaction products are reported (*vide infra)..*

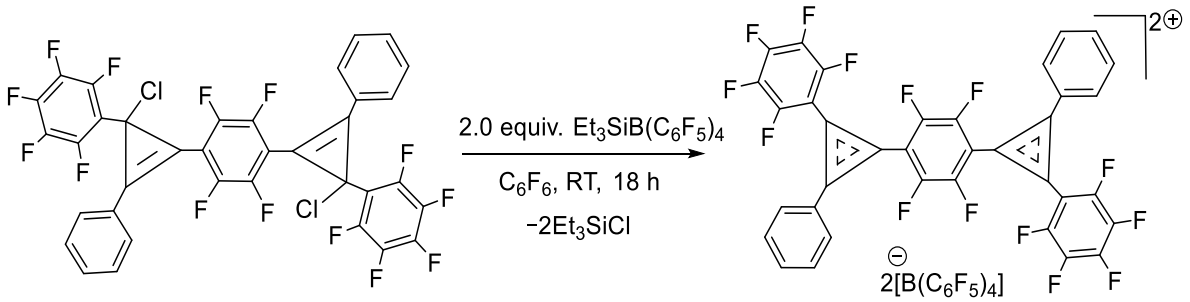
Synthesis 6



6 was prepared by following the protocol for **1** whereas 1,4-bis(3-chloro-2,3-diphenyl-1-cyclopropene)-2,3,5,6,-tetrafluorobenzene (59.9 mg, 0.10 mmol, 1.0 equiv.), $Et_3Si[B(C_6F_5)_4]$ (158.0 mg, 0.20 mmol, 2.0 equiv.) were employed in toluene (4.0 mL). After stirring at RT for 18 h, the toluene layer was pipetted out. The residue was washed with *n*-hexane (3 x 3 mL) followed by drying afforded yellow powder compound **6** (168 mg, 89%). *X*-ray quality crystals were grown with the mixture of solvents using DCM:CH_3CN:*n*-hexanes (1:1:5) at RT for a week. **6**: $C_{84}H_{20}B_2F_{44}$ requires: C 53.5, H 1.07. Found: C 53.4, H 1.68%. ^{1}H NMR (400 MHz, CD_3CN): δ_H 8.65 (dt, *J* = 8.3, 1.8 Hz, 8 H, Ar-*H*), 8.17 (tt, *J* = 7.7, 1.5 Hz, 4 H, Ar-*H*), 8.05 - 7.92 (m, 8 H, Ar-*H*); ^{19}F NMR (377 MHz, CD_3CN): δ_F -126.6 (s, 4 F, C_6F_4), -133.8 (m, 16 F, *o*-C_6F_5 of -$B(C_6F_5)_4$), -163.9 (m, 8 F, *p*-C_6F_5 of -$B(C_6F_5)_4$), -168.3 (m, 16 F, *m*-C_6F_5 of -$B(C_6F_5)_4$); ^{11}B NMR (128 MHz, CD_3CN): δ_B -16.7 (br s, 2 B, -*B*$(C_6F_5)_4$); ^{13}C NMR (101 MHz,

CD_3CN): δ_C 160.1 (s, $Ar_3C_3)^+$, 150.4 (br m, -C_6F_5), 148.0 (br m, -C_6F_5), 141.5 (s, C_{Ar} of Ph), 140.6 (br m, -C_6F_5), 138.6 (br m, -C_6F_5), 138.1 (s, C_{Ar} of Ph), 136.1 (br m, -C_6F_4-), 131.9 (s, C_{Ar} of Ph), 120.2 (C_{Ar} of Ph). Efforts to obtain EA or HRMS ddata for this highly Lewis acidic dication were unnssccessful. Nonetheless, full characterization of subsequent reaction products are reported (*vide infra).*.

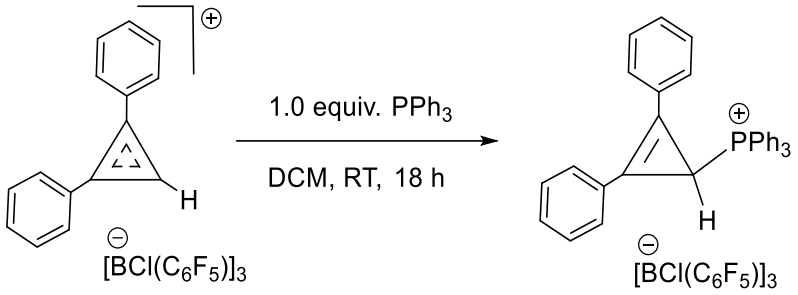
Synthesis 7



7 was prepared by following the protocol for **1** whereas 1,4-bis(3-chloro-2-phenyl-3-pentaflurophenyl-1-cyclopropene)-2,3,5,6,-tetrafluorobenzene (77.9 mg, 0.10 mmol, 1.0 equiv.), $Et_3Si[B(C_6F_5)_4]$ (158.0 mg, 0.20 mmol, 2.0 equiv.) were employed in C_6F_6 (4.0 mL). After stirring at RT for 18 h, the C_6F_6 layer was pipetted out. The residue was washed with *n*-hexane (3 x 3 mL) followed by drying afforded dark-brown powder compound **7** (161 mg, 78%). Crystals were grown with the mixture of solvents using DCM:PhCN:*n*-hexanes (1:1:5) at RT for a week and data was not publishable quality but confirms the molecular architecture. **7:** ^{1}H NMR (400 MHz, CD_3CN): δ_H 8.62 (dt, *J* = 8.3, 1.1 Hz, 4 H, Ar-*H*), 8.23 (tt, *J* = 7.6, 1.1 Hz, 2 H, Ar-*H*), 8.06 - 7.94 (m, 4 H, Ar-*H*); ^{19}F NMR (377 MHz, CD_3CN): δ_F -126.9 (s, 4 F, -C_6F_4-), -132.1 (m, 4 F, *o*-C_6F_5 of (-$(C_6F_5)PhC_3)^+$), -133.8 (m, 16 F, *o*-C_6F_5 of -$B(C_6F_5)_4$), -141.1 (m, 2 F, *p*-C_6F_5 of (-$(C_6F_5)PhC_3)^+$), -158.5 (m, 4 F, *m*-C_6F_5 of (-$(C_6F_5)PhC_3)^+$), -164.0 (m, 8 F, *p*-C_6F_5 of -$B(C_6F_5)_4$), -168.4 (m, 16 F, *m*-C_6F_5 of -$B(C_6F_5)_4$); ^{11}B NMR (128 MHz, CD_3CN): δ_B -16.7 (br s, 2 B, -$B(C_6F_5)_4$); ^{13}C NMR (101 MHz, CD_3CN): δ_C 159.9 (s, $Ar_3C_3)^+$, 150.2 (br m, -C_6F_5), 147.9 (br m, -C_6F_5), 146.6 (br m, -C_6F_5), 146.2 (br m, -C_6F_5), 143.0 (s, C_{Ar} of Ph), 140.6 (br m, -C_6F_5), 139.1 (s, C_{Ar} of Ph), 138.6 (br m, -C_6F_5), 138.6 (br m, -C_6F_5), 136.1 (br m, -C_6F_4-), 131.8 (s, C_{Ar} of Ph), 119.1 (C_{Ar} of Ph). Efforts to

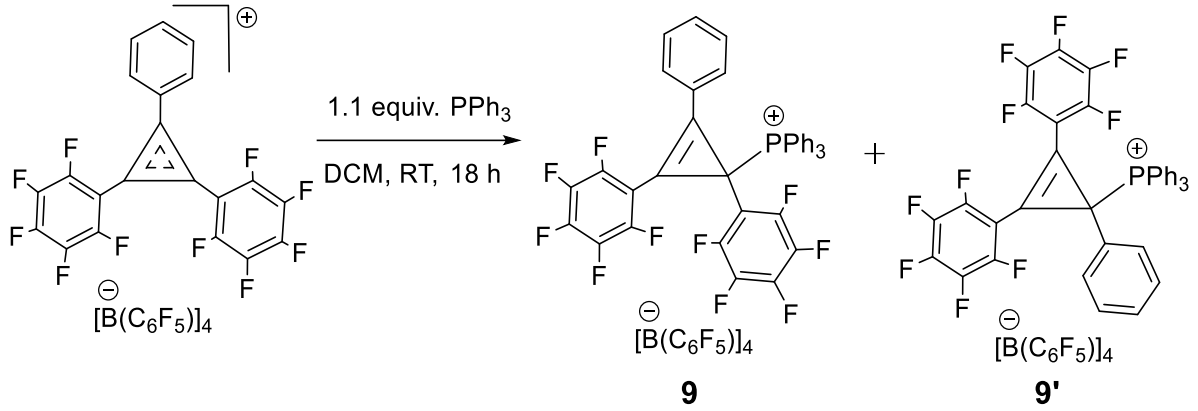
obtain EA or HRMS ddata for this highly Lewis acidic dication were unnssccessful. Nonetheless, full characterization of subsequent reaction products are reported (*vide infra)..*

Synthesis 8



Into a 4 mL vial equipped with a stir bar, $[(Ph_2C)_2CH][ClB(C_6F_5)_3]$, **1** (36.9 mg, 0.05 mmol, 1.0 equiv.) was taken in DCM (0.5 mL). A solution of PPh_3 (15.7 mg, 0.06 mmol, 1.1 equiv.) in DCM (0.5 mL) was transferred to the vial. The reaction mixture was allowed to stir at RT for 18 h. After removal of all volatiles, the residue was washed with *n*-hexane (3 x 1 mL) and followed by drying afforded compound **8** (48.0 mg, 96%). *X*-ray quality crystals were grown with a mixture of solvent of DCM:*n*-hexane (1:5) at RT for a week. **8**: $C_{51}H_{26}BClF_{14}P{\cdot}CH_2Cl_2$ requires: C 57.5, H 2.60. Found: C 57.6, H 2.07%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.83 - 7.72 (m, 3 H, Ar-*H*), 7.78 - 7.54 (m, 12 H, Ar-*H*), 7.43 - 7.30 (m, 10 H, Ar-*H*), 3.77 (d, $^1J_{H\text{-}P}$ = 48 Hz,1 H, $(Ph_2C)_2C$*H*-PPh_3); ^{31}P NMR (162 MHz, $CDCl_3$): δ_P 22.5 (d, $^1J_{P\text{-}H}$ = 48 Hz,1 P, $(Ph_2C)_2$CH-*P*Ph_3); ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$): δ_P 22.5 (s, 1 P, $(Ph_2C)_2$CH-*P*Ph_3); ^{19}F NMR (377 MHz, $CDCl_3$): δ_F -132.0 (m, 6 F, *o*-C_6F_5 of -$BCl(C_6F_5)_3$), -161.6 (m, 3 F, *p*-C_6F_5 of -$BCl(C_6F_5)_3$), -166.4 (m, 6 F, *m*-C_6F_5 of -$BCl(C_6F_5)_3$); ^{11}B NMR (128 MHz, $CDCl_3$): δ_B -6.9 (br s, 1 B, -*B*$Cl(C_6F_5)_3$); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 149.5 (br m, -*C*$_6F_5$), 147.0 (br m, -*C*$_6F_5$), 140.1 (br m, -*C*$_6F_5$), 137.8 (br m, -*C*$_6F_5$), 135.4 (d, $J_{C\text{-}P}$ = 3.3 Hz, C_{Ar}), 134.4 (br m, -*C*$_6F_5$), 133.6 (d, $J_{C\text{-}P}$ = 9.9 Hz, C_{Ar}), 131.1 (s, C_{Ar}), 130.5 (d, $J_{C\text{-}P}$ = 11.6 Hz, C_{Ar}), 129.4 (d, $J_{C\text{-}P}$ = 16.2 Hz, C_{Ar}), 125.2 (d, $J_{C\text{-}P}$ = 3.2 Hz, C_{Ar}), 118.6 (d, $J_{C\text{-}P}$ = 87.0 Hz, C_{Ar}), 105.4 (d, $J_{C\text{-}P}$ = 2.2 Hz, $(Ph_2C)_2$CH-PPh_3), 16.8 (d, $J_{C\text{-}P}$ = 73.1 Hz, $(Ph_2C)_2$*C*H-PPh_3). HRMS (ESI, Positive): m/z: 453.1761 (M^+) (calcd.: 453.1767 for $C_{33}H_{26}P^+$).

Synthesis 9 and 9′

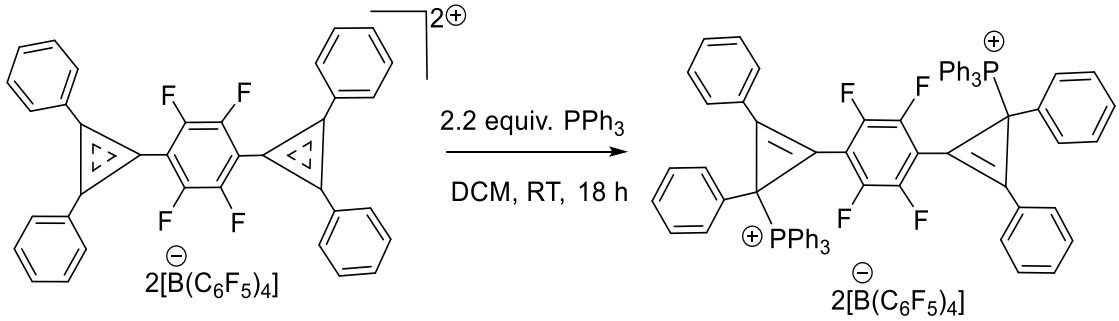


9 **9'**

Compounds **9** and **9′** were prepared by following the protocol for **8** whereas $[Ph(C_6F_5)_2C_3][B(C_6F_5)_4]$ (**3**) (56.3 mg, 0.05 mmol, 1.0 equiv.), PPh_3 (15.7 mg, 0.06 mmol, 1.1 equiv.) were employed in DCM (1.0 mL). After work up, it gave mixture of compounds **9** and **9′** in a total yield of 58.0 mg, 84%. The salts were inseperable mixture whilst ^{31}P NMR suggests **9** and **9′** is 1:1. *X*-ray quality crystals were grown with a mixture of solvent of DCM:PhCN:*n*-hexanes (1:1:5) at RT for a week. **9** and **9′**: ^{1}H NMR (400 MHz, CD_3CN/DCM): δ_H 8.24 - 8.03 (m, 13 H, Ar-*H*), 8.03 - 7.92 (m, 4H, Ar-*H*), 7.92 - 7.80 (m, 3 H, Ar-*H*); ^{31}P NMR (162 MHz, CD_3CN/DCM): δ_P 25.8 (s, 1 P, $(Ph(C_6F_5)C)_2C(C_6F_5)$-*P*Ph_3), 25.1 (s, 1 P, $((C_6F_5)_2C)_2C(Ph)$-*P*Ph_3); $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_3CN/DCM): δ_P 25.8 (s, 1 P, $(Ph(C_6F_5)C)_2C(C_6F_5)$-*P*Ph_3), 25.1 (s, 1 P, $((C_6F_5)_2C)_2C(Ph)$-*P*Ph_3); ^{19}F NMR (377 MHz, CD_3CN/DCM): δ_F -133.7 (m, 8 F, *o*-C_6F_5 of -$B(C_6F_5)_4$), -135.9 (m, 4 F, *o*-C_6F_5 of $((C_6F_5)_2C)_2C(Ph)$-PPh_3), -136.3 (m, 2 F, *o*-C_6F_5 of $(Ph(C_6F_5)C)_2C(C_6F_5)$-PPh_3), -137.8 (m, 2 F, *o*-C_6F_5 of $(Ph(C_6F_5)C)_2C(C_6F_5)$-PPh_3), -145.2 (m, 2 F, *p*-C_6F_5 of $((C_6F_5)_2C)_2C(Ph)$-PPh_3), -147.2 (m, 1 F, *p*-C_6F_5 of $(Ph(C_6F_5)C)_2C(C_6F_5)$-PPh_3), -150.2 (m, 1 F, *p*-C_6F_5 of $(Ph(C_6F_5)C)_2C(C_6F_5)$-PPh_3), -159.7 (m, 4 F, *m*-C_6F_5 of $((C_6F_5)_2C)_2C(Ph)$-PPh_3), -160.1 (m, 2 F, *m*-C_6F_5 of $(Ph(C_6F_5)C)_2C(C_6F_5)$-PPh_3), -160.6 (m, 2 F, *m*-C_6F_5 of $(Ph(C_6F_5)C)_2C(C_6F_5)$-PPh_3), -164.6 (m, 4 F, *p*-C_6F_5 of -$B(C_6F_5)_4$), -168.4 (m, 8 F, *m*-C_6F_5 of -$B(C_6F_5)_4$); ^{11}B NMR (128 MHz, CD_3CN/DCM): δ_B -17.9 (br s, 1 B, -*B*$(C_6F_5)_4$); ^{13}C NMR (101 MHz, CD_3CN/DCM): δ_C 150.2 (br m, -*C*$_6F_5$), 147.8 (br m, -*C*$_6F_5$), 146.3 (br m, -*C*$_6F_5$), 145.6 (br m, -*C*$_6F_5$), 143.7 (br m, -*C*$_6F_5$), 140.1 (br m, -*C*$_6F_5$), 139.5 (br m, -*C*$_6F_5$), 138.1 (br m, -*C*$_6F_5$), 137.7 (br m, -*C*$_6F_5$),

137.0 (br m, -C_6F_5), 135.9 (m, C_{Ar}), 135.7 (br m, -C_6F_5), 134.7 (d, J_{C-P} = 9.4 Hz, C_{Ar}), 134.5 (d, J_{C-P} = 10.1 Hz, C_{Ar}), 133.2 (s, C_{Ar}), 132.3 (d, J_{C-P} = 29.0 Hz, C_{Ar}), 130.4 (d, J_{C-P} = 12.1 Hz, C_{Ar}), 130.1 (d, J_{C-P} = 12.8 Hz, C_{Ar}), 129.7 (d, J_{C-P} = 16.2 Hz, C_{Ar}), 129.0 (s, C_{Ar}), 117.0 (d, J_{C-P} = 83.9 Hz, C_{Ar}), 116.5 (d, J_{C-P} = 83.9 Hz, C_{Ar}), doublets are not resolved for -C(Ph)-PPh_3 and -C(C_6F_5)-PPh_3. HRMS (ESI, Positive) m/z: 709.1130 (M^+) (calcd.: 709.1137 for $C_{39}H_{20}F_{10}P^+$).

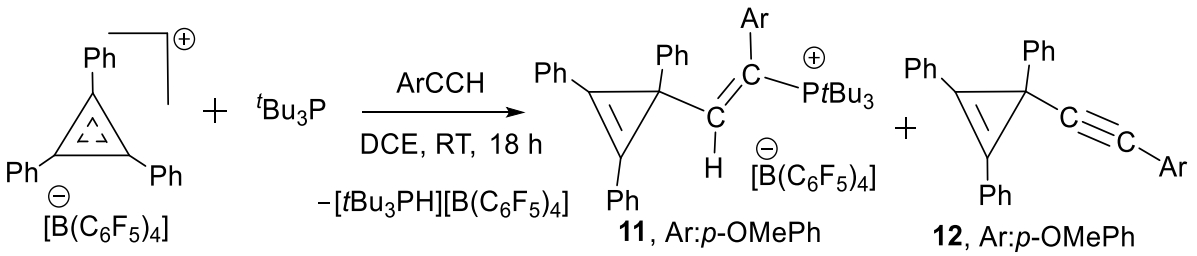
Synthesis 10



Compounds **10** was prepared by following the protocol for **8** whereas [Ph_2C_3-C_6F_4-C_3Ph_2][2B(C_6F_5)$_4$] (**6**) (56.6 mg, 0.03 mmol, 1.0 equiv.), PPh_3 (18.4 mg, 0.07 mmol, 2.2 equiv.) were employed in DCM (1.0 mL). After work up, it gave compound **10** (70.0 mg, 97%). *X*-ray quality crystals were grown with a mixture of solvent of DCM:CH_3CN:*n*-hexanes (1:1:5) at -30 ^oC for a week. **10**: $C_{120}H_{50}B_2F_{44}P_2$·2.7$CH_2Cl_2$ requires: C 55.8, H 2.11. Found: C 55.8, H 2.33%. ^{1}H NMR (400 MHz, CD_3CN/DCM): δ_H 7.85 - 7.74 (m, 6 H, Ar-*H*), 7.63 - 7.52 (m, 25 H, Ar-*H*), 7.49 - 7.43 (m, 8 H, Ar-*H*), 7.41 - 7.35 (m, 3 H, Ar-*H*), 7.34 - 7.27 (m, 4 H, Ar-*H*), 7.28 - 7.21 (m, 4 H, Ar-*H*); ^{31}P NMR (162 MHz, CD_3CN/DCM): δ_P 30.8 (s, 1 P, -(C_6F_4)C_3(Ph_2)*P*Ph_3); ^{31}P{^{1}H} NMR (162 MHz, CD_3CN/DCM): δ_P 30.8 (s, 1 P, -(C_6F_4)C_3(Ph_2)*P*Ph_3); ^{19}F NMR (377 MHz, CD_3CN/DCM): δ_F -133.5 (m, 8 F, *o*-C_6F_5 of -B(C_6F_5)$_4$), -135.0 (d, J_{F-F} = 39.7 Hz, 4 F, C_6F_4 of (PPh_3(Ph_2)C_3(C_6F_4)C_3(Ph_2)PPh_3)), -163.8 (m, 4 F, *p*-C_6F_5 of -B(C_6F_5)$_4$), -168.1 (m, 8 F, *m*-C_6F_5 of -B(C_6F_5)$_4$); ^{11}B NMR (128 MHz, CD_3CN/DCM): δ_B -16.7 (br s, 1 B, -*B*(C_6F_5)$_4$); ^{13}C NMR (101 MHz, CD_3CN/DCM): δ_C 150.2 (br m, -C_6F_5), 147.7 (br m, -C_6F_5), 140.2 (br m, -C_6F_5), 138.2 (br m, -C_6F_5), 137.8 (br m, -C_6F_5), 137.5 (br m, -C_6F_5), 136.1 (d, J_{C-P} = 3.3 Hz, C_{Ar}), 135.6 (d, J_{C-P} = 2.5 Hz, C_{Ar}), 135.5 (d, J_{C-P} = 2.3 Hz, C_{Ar}), 133.3 (s, C_{Ar}), 131.0 (d, J_{C-P} = 12.4 Hz, C_{Ar}), 130.8 (s, C_{Ar}), 130.2 (d, J_{C-P}

= 24.0 Hz, C_{Ar}), 129.7 (s, C_{Ar}), 129.0 (d, $J_{C\text{-}P}$ = 3.4 Hz, C_{Ar}), 124.6 (s, C_{Ar}), 119.7 (s, C_{Ar}), 118.7 (d, $J_{C\text{-}P}$ = 83.4 Hz, C_{Ar}), 33.9 (d, $J_{C\text{-}P}$ = 74.0 Hz, (-*C*(Ph)-PPh_3). MS (MALDI-TOF) m/z: 528.2 (M^+-2PPh_3) (calcd.: 528.1 for $C_{36}H_{20}F_4^{2+}$).

Synthesis 11 and 12



Into a 4 mL vial equipped with a stir bar, $[Ph_3C_3][B(C_6F_5)_4]$, **2a** (94.6 mg, 0.1 mmol, 1.0 equiv.) and *t*Bu_3P (20.2 mg, 0.10 mmol, 1.0 equiv.) were taken in DCE (1.0 mL). A solution of 4-methoxy phenylacetylene (13.2 mg, 0.1 mmol, 1.0 equiv.) in DCE (0.5 mL) was transferred to the vial. The reaction mixture was allowed to stir at RT for 18 h. ^{31}P NMR analysis of the crude mixture suggests $[tBu_3PH][B(C_6F_5)_4]$ (80% yield), $[(Ph_3C)_3CHC(C_6H_4OMe)P(t\text{-}Bu)_3][B(C_6F_5)_4]$] (**11**) (20% yield) and affirms completion of reaction. After removal of all volatiles, the residue was extracted with benzene (3 x 2 mL) and the benzene washings were combined together for chromatographic purification.

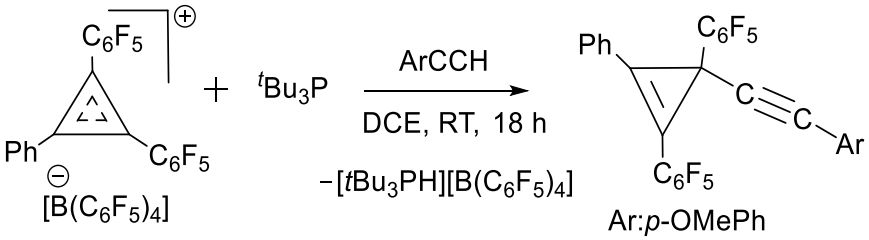
The oily residue, a mixture of salts, was crystalized in DCM:*n*-hexane (1:5) at RT for a week. Since the salts were inseperable mixture, a partial characterization data included here for **11**.

11: ^{31}P NMR (162 MHz, DCM): δ_P 45.5 (m, 1 P, -$(Ph_3C)_3CHC(Ar)P(t\text{-}Bu)_3$), $^{31}P\{^1H\}$ NMR (162 MHz, DCM): δ_P 45.5 (s, 1 P, -$(Ph_3C)_3CHC(Ar)P(t\text{-}Bu)_3$); ^{19}F NMR (377 MHz, DCM): δ_F -132.4 (m, 8 F, *o*-C_6F_5 of -$B(C_6F_5)_4$), -162.8 (m, 4 F, *p*-C_6F_5 of -$B(C_6F_5)_4$), -166.6 (m, 8 F, *m*-C_6F_5 of -$B(C_6F_5)_4$); ^{11}B NMR (128 MHz, DCM): δ_B -16.6 (br s, 1 B, -$B(C_6F_5)_4$). HRMS (ESI, Positive) m/z: 601.3595 (M^+) (calcd.: 601.3594 for $C_{42}H_{50}OP^+$).

Combined benzene washings were taken and all volatiles were evaporated off under reduced pressure. The residue was taken into minimum DCM. The DCM solution loaded on preparative TLC plates and eleuted with 10% EtOAc and *n*-hexanes. This yielded a major

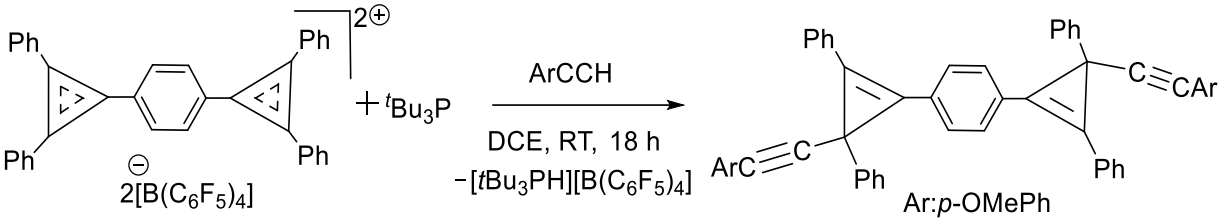
yellow band with the R_f = 0.53. This was collected in affording yellow solid compound **12** (29.0 mg, 73%). *X*-ray quality crystals were grown via evaporation of a $CDCl_3$ solution of **12**. **12**: ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.75 (dt, *J* = 7.6, 1.3 Hz, 4 H, Ar-*H*), 7.60 (dt, *J* = 7.7, 1.4 Hz, 2 H, Ar-*H*), 7.52 - 7.43 (m, 4 H, Ar-*H*), 7.44 - 7.34 (m, 4 H, Ar-*H*), 7.30 (tt, *J* = 7.9, 1.7 Hz, 2 H, Ar-*H*), 7.18 (tt, *J* = 7.3, 1.8 Hz, 1 H, Ar-*H*), 6.81 (dt, *J* = 8.8, 1.8 Hz, 2 H, Ar-*H*), 3.79 (s, 1 H, -OC*H*$_3$); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 159.2 (s, *C*$_{Ar}$ of Ph), 142.9 (s, *C*$_{Ar}$ of Ph), 133.3 (s, *C*$_{Ar}$ of Ph), 130.1 (s, *C*$_{Ar}$ of Ph), 129.4 (s, *C*$_{Ar}$ of Ph), 129.1 (s, *C*$_{Ar}$ of Ph), 128.2 (s, *C*$_{Ar}$ of Ph), 126.7 (s, *C*$_{Ar}$ of Ph), 126.3 (s, *C*$_{Ar}$ of Ph), 125.9 (s, *C*$_{Ar}$ of Ph), 116.4 (s, *C*$_{Ar}$ of Ph), 113.9 (s, *C*$_{Ar}$ of Ph), 112.5 (s, (Ph$_2$*C*)$_2$C(Ph)-), 90.8 (s, *C*$_{alkyne}$), 78.4 (s, *C*$_{alkyne}$), 55.4 (s, -O*C*H$_3$), 24.0 (s, (Ph$_2$C)$_2$*C*(Ph)-). HRMS (DART) m/z: 399.1737 (M^++H) (calcd.: 399.1743 for $C_{30}H_{23}O$).

Synthesis 13



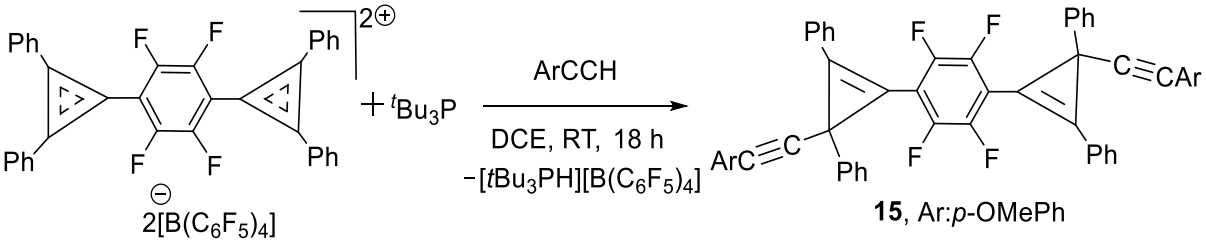
13 (39 mg, 67%) was prepared by following the protocol for **12**. **13**: ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.94 (dt, *J* = 7.7, 1.5 Hz, 2 H, Ar-*H*), 7.59 - 7.45 (m, 2 H, Ar-*H*), 7.50 (tt, *J* = 7.9, 1.9 Hz, 1 H, Ar-*H*), , 7.39 - 7.28 (m, 2 H, Ar-*H*), 6.87 - 6.67 (m, 2 H, Ar-*H*), 3.78 (s, 1 H, -OC*H*$_3$); ^{19}F NMR (377 MHz, $CDCl_3$): δ_F -136.7 (m, 2 F, *o*-C$_6$*F*$_5$ of -C(C$_6$*F*$_5$)-CCAr), -141.4 (m, 2 F, *o*-C$_6$*F*$_5$ of ((C$_6$*F*$_5$)(Ph)C)$_2$C-), -151.0 (m, 1 F, *p*-C$_6$*F*$_5$ of -C(C$_6$*F*$_5$)-CCAr), -156.2 (m, 1 F, *p*-C$_6$*F*$_5$ of ((C$_6$*F*$_5$)(Ph)C)$_2$C-), -161.0 (m, 2 F, *m*-C$_6$*F*$_5$ of -C(C$_6$*F*$_5$)-CCAr), -162.0 (m, 2 F, *m*-C$_6$*F*$_5$ of ((C$_6$*F*$_5$)(Ph)C)$_2$C-); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 159.8 (s, *C*$_{Ar}$ of Ph), 146.4 (br s, -*C*$_6$F$_5$), 143.8 (br s, -*C*$_6$F$_5$), 139.4 (br m, -*C*$_6$F$_5$), 136.6 (br m, -*C*$_6$F$_5$), 134.6 (br m, -*C*$_6$F$_5$), 133.6 (s, *C*$_{Ar}$ of Ph), 131.2 (s, *C*$_{Ar}$ of Ph), 130.2 (s, *C*$_{Ar}$ of Ph), 130.0 (br m, *C*$_{Ar}$ of Ph), 128.5 (s, *C*$_{Ar}$ of Ph), 126.4 (s, *C*$_{Ar}$ of Ph), 125.2 (s, *C*$_{Ar}$ of Ph), 121.0 (Ph(C$_6$F$_5$)*C*)$_2$C-), 115.1 (Ph(C$_6$F$_5$)*C*)$_2$C-)), 114.0 (s, *C*$_{Ar}$ of Ph), 89.1 (s, *C*$_{alkyne}$), 80.9 (s, *C*$_{alkyne}$), 55.5 (s, -O*C*H$_3$), 31.1 (s, -*C*(C$_6$F$_5$)-CCAr). HRMS (DART) m/z: 579.07939 (M^++H) (calcd.: 579.08012 for $C_{30}H_{13}OF_{10}$).

Synthesis 14



14 (25 mg, 69%) was prepared by following the protocol for **12** whereas $[Ph_2C_3C_6H_4C_3Ph_2][2B(C_6F_5)_4]$ (**5**) (90.7 mg, 0.05 mmol, 1.0 equiv.), *t*Bu_3P (20.2 mg, 0.10 mmol, 2.0 equiv.) and 4-methoxy phenylacetylene (13.2 mg, 0.1 mmol, 2.0 equiv.) were employed in DCE (1.5 mL). **14**: ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.81 (s, 4 H, -$C_3C_6H_4C_3$-), 7.69 - 7.63 (m, 4 H, Ar-*H*), 7.56 (tt, *J* = 7.2, 1.4 Hz, 4 H, Ar-*H*), 7.49 - 7.43 (m, 8 H, Ar-*H*), 7.41 - 7.37 (m, 8 H, Ar-*H*), 6.82 - 6.79 (m, 4 H, Ar-*H*), 3.79 (s, 6 H, -OCH_3); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 159.2 (s, C_{Ar} of Ph), 144.8 (s, C_{Ar} of Ph), 142.6 (s, C_{Ar} of Ph), 133.3 (s, C_{Ar} of Ph), 130.5 (s, C_{Ar} of Ph), 130.2 (s, C_{Ar} of Ph), 130.1 (s, C_{Ar} of Ph), 129.1 (s, C_{Ar} of Ph), 129.2 (s, C_{Ar} of Ph), 128.3 (s, C_{Ar} of Ph), 128.2 (s, C_{Ar} of Ph), 127.0 (s, C_{Ar} of Ph),126.3 (s, C_{Ar} of Ph), 116.5 (-$C_3C_6H_4C_3$-), 116.2 (-$C_3C_6H_4C_3$-), 113.9 (s, C_{Ar} of Ph), 90.7 (s, C_{alkyne}), 78.6 (s, C_{alkyne}), 55.4 (s, -OCH_3), 29.7 (s, -*C*(Ph)-CCAr). HRMS (DART) m/z: 719.29404 (M^++H) (calcd.: 719.29446 for $C_{54}H_{39}O_2$).

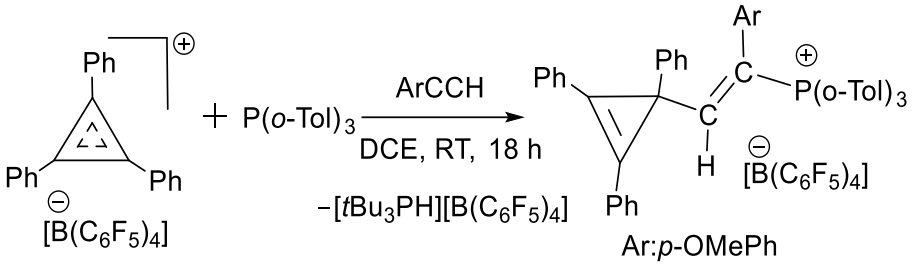
Synthesis 15



15 (26 mg, 66%) was prepared by following the protocol for **12** whereas $[Ph_2C_3C_6F_4C_3Ph_2][2B(C_6F_5)_4]$ (**6**) (94.3 mg, 0.05 mmol, 1.0 equiv.), *t*Bu_3P (20.2 mg, 0.10 mmol, 2.0 equiv.) and 4-methoxy phenylacetylene (13.2 mg, 0.1 mmol, 2.0 equiv.) were employed in DCE (1.5 mL). **15**: ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.95 - 7.78 (m, 8 H, Ar-*H*), 7.58 - 7.50 (m, 4 H, Ar-*H*), 7.48 - 7.43 (m, 4 H, Ar-*H*), 7.43 - 7.39 (m, 4 H, Ar-*H*), 7.30 - 7.26 (m, 4 H, Ar-*H*), 6.82 - 7.79 (m, 4 H, Ar-*H*), 3.79 (s, 6 H, -OCH_3);^{19}F NMR (377 MHz, $CDCl_3$): δ_F -138.5 (s, 4 F,-$C_3C_6H_4C_3$-); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 159.5 (s, C_{Ar} of Ph), 143.8 (br

m, C_{Ar} of C_6F_4), 133.5 (s, C_{Ar} of Ph), 131.2 (s, C_{Ar} of Ph), 130.8 (s, C_{Ar} of Ph), 129.9 (s, C_{Ar} of Ph), 129.6 (s, C_{Ar} of Ph), 129.5 (s, C_{Ar} of Ph), 129.3 (s, C_{Ar} of Ph), 128.9 (s, C_{Ar} of Ph), 128.4 (s, C_{Ar} of C_6F_4), 127.1 (s, C_{Ar} of Ph), 126.5 (s, C_{Ar} of Ph), 126.4 (s, C_{Ar} of Ph), 125.7 (s, C_{Ar} of Ph), 116.0 (-$C_3C_6H_4C_3$-), 115.9 (-$C_3C_6H_4C_3$-), 90.2 (s, C_{alkyne}), 79.5 (s, C_{alkyne}), 55.5 (-OCH_3), 29.8 (s, -*C*(Ph)-CCAr). HRMS (DART) m/z: 791.25856 (M^++H) (calcd.: 791.25677 for $C_{54}H_{35}O_2F_4$).

Synthesis 16

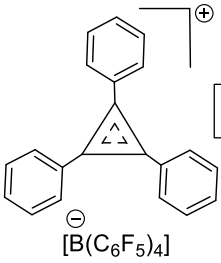


16 (89.9 mg, 65%) was prepared by following the protocol for **11** whereas $[Ph_3C_3][B(C_6F_5)_4]$ (**2a**) (19.2 mg, 0.02 mmol, 1.0 equiv.), P(*o*-Tol)$_3$ (20.2 mg, 0.02 mmol, 1.0 equiv.) and 4-methoxy phenylacetylene (13.2 mg, 0.1 mmol, 1.0 equiv.) were employed in DCE (1.5 mL). ^{31}P NMR suggests **16** (65% yield) and $[HP(o\text{-Tol})_3][B(C_6F_5)_4]$ (35% yield). **16**: ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 7.69 (tt, *J* = 7.9, 1.2 Hz, 1 H, Ar-*H*), 7.64 - 7.51 (m, 2 H, Ph*H*), 7.47 (tt, *J* = 6.9, 1.1 Hz, 2 H, Ar-*H*), 7.43 - 7.27 (m, 11 H, Ph*H*), 7.23 - 7.14 (m, 4 H, Ph*H*), 7.14 - 6.96 (m, 9 H, Ph*H*), 6.95 7.14 - 6.78 (m, 2 H, Ph*H*), 6.39 (s, 1 H, C*H*=*C*), 3.43 (s, 3 H, -OCH_3), 2.68 (br s, 3 H, -CH_3 of P(*o*-Tol)$_3$), 2.28 (s, 3 H, -CH_3 of P(*o*-Tol)$_3$), 1.56 (br s, 3 H, -CH_3 of P(*o*-Tol)$_3$); ^{31}P NMR (400 MHz, $CDCl_3$): δ_P 28.3 (s, 1 P of -C=C-*P*(*o*-Tol)$_3$-), ^{31}P{^{1}H} NMR (400 MHz, $CDCl_3$): δ_P 28.3 (s, 1 P of -C=C-*P*(*o*-Tol)$_3$-); ^{19}F NMR (400 MHz, $CDCl_3$): δ_F -132.5 (m, 8 F, *o*-C_6F_5 of -B(C_6F_5)$_4$), -163.2 (m, 4 F, *p*-C_6F_5 of -B(C_6F_5)$_4$), -166.9 (m, 8 F, *m*-C_6F_5 of -B(C_6F_5)$_4$); ^{11}B NMR (128 MHz, $CDCl_3$): δ_B 16.6 (br s, 1 B); ^{13}C NMR (126 MHz, $CDCl_3$): δ_C 160.6 (s, C_{Ar} of Ph), 149.7 (br m, C_{Ar} of C_6F_4), 147.2 (br m, C_{Ar} of C_6F_4), 139.7 (br m, C_{Ar} of C_6F_4), 137.7 (br m, C_{Ar} of C_6F_4), 134.5 (br m, C_{Ar} of C_6F_4), 134.6 (d, *J* = 13.6 Hz, C_{Ar} of Ph), 133.8 (s, C_{Ar} of Ph), 133.4 (d, *J* = 7.7 Hz, C_{Ar} of Ph), 130.5 (s, C_{Ar} of Ph), 130.1 (s, C_{Ar} of Ph),

130.0 (s, C_{Ar} of Ph), 129.6 (s, C_{Ar} of Ph), 129.5 (s, C_{Ar} of Ph), 129.1 (d, J = 9.7 Hz, C_{Ar} of Ph), 129.0 (s, C_{Ar} of Ph), 128.8 (s, C_{Ar} of Ph), 128.6 (s, C_{Ar} of Ph), 128.4 (s, C_{Ar} of Ph), 128.2 (s, C_{Ar} of Ph), 127.0 (s, C_{Ar} of Ph), 126.7 (s, C_{Ar} of Ph) 126.1 (s, C_{Ar} of Ph), 114.4 (-C_2(Ph_2)), 114.1 (s, C_{Ar} of Ph), 75.9 (P-C=CH), 55.2 (-O$C$$H_3$), 29.1 (s, -$C$(Ph)-CH=C). HRMS (ESI, Positive) m/z: 703.3122 for [M^+] (calcd.: 703.3124 for $C_{51}H_{44}OP$).

Cyclic Voltammetry (CV) data for all compounds

Compound 2a



E_{Red} = (0.676+0.002) V = 0.69 V

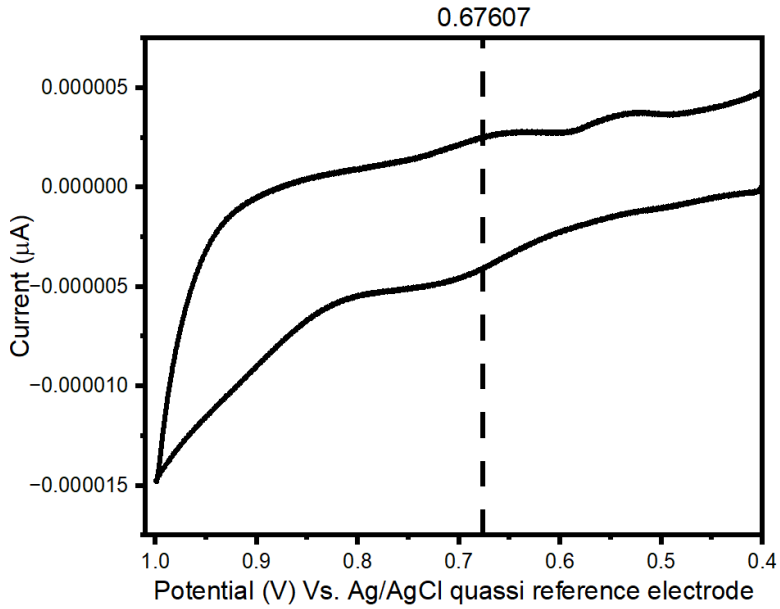


Figure S1. Evolution of CV of **2a** (0.1 M) in CH_3CN/DCM (1:1) with $[(n\text{-}Bu)_4N]PF_6$ as supporting electrolyte. Scan rate employed: 0.1 V s^{-1}.

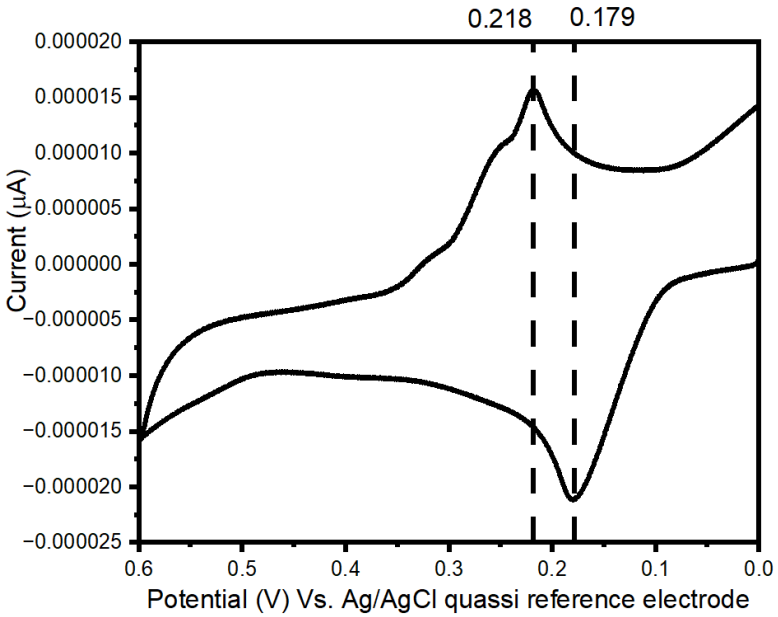
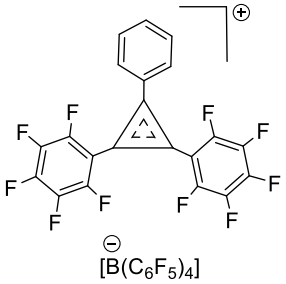


Figure S2. Evolution of CV of **2a** with internal ferrocene standard.

Compound 3



E_{Red} = (0.498+0.074) V = 0.57 V

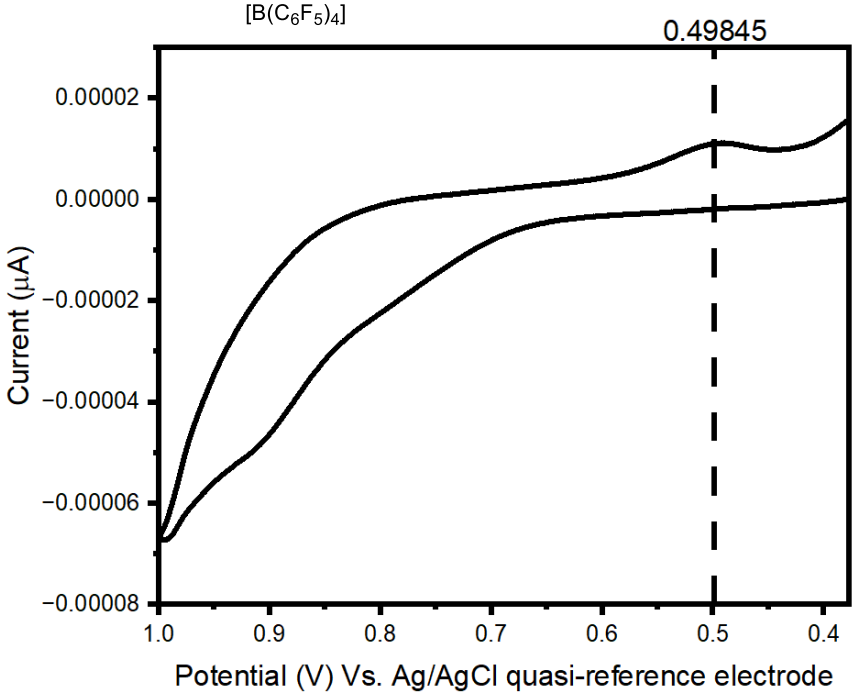


Figure S3. Evolution of CV of **3** (0.1 M) in CH_3CN/DCM (1:1) with $[(n\text{-}Bu)_4N]PF_6$ as supporting electrolyte. Scan rate employed: 0.1 V s^{-1}.

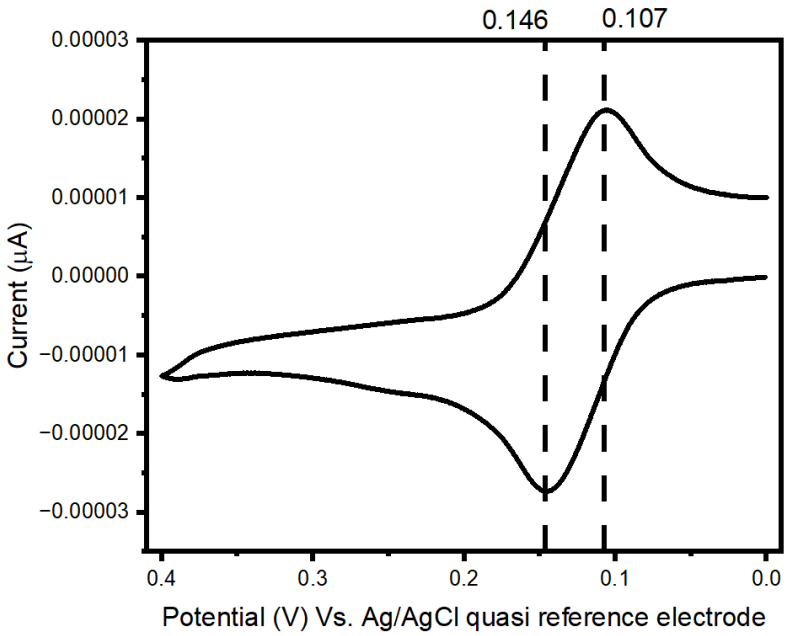
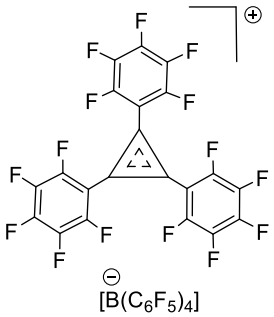


Figure S4. Evolution of CV of **3** with internal ferrocene standard.

Compound 4a



E_{Red} = (0.418+0.038) V = 0.47 V

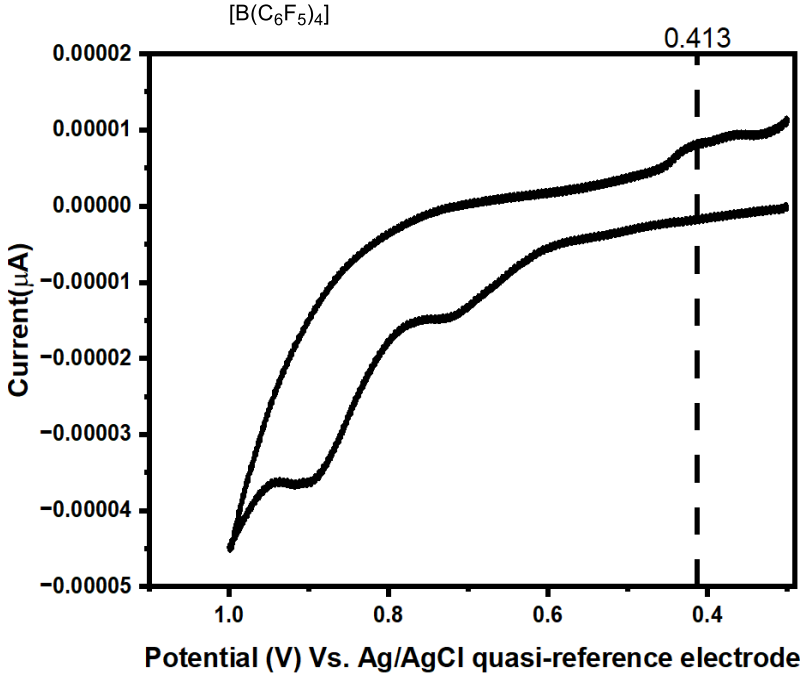


Figure S5. Evolution of CV of **4a** (0.1 M) in CH_3CN/DCM (1:1) with [(*n*-Bu)$_4$N]PF_6 as supporting electrolyte. Scan rate employed: 0.1 V s^{-1}.

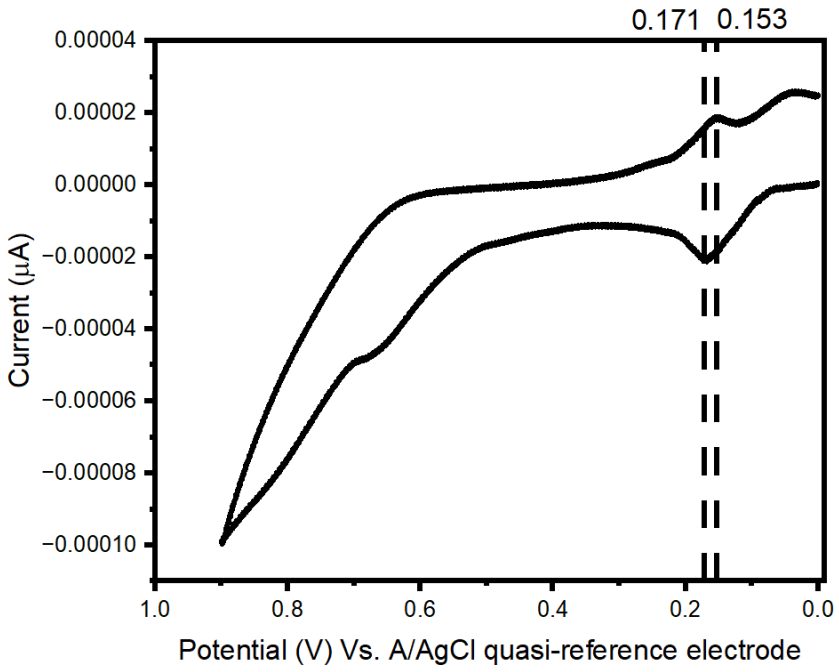


Figure S6. Evolution of CV of **4a** with internal ferrocene standard.

Compound 5

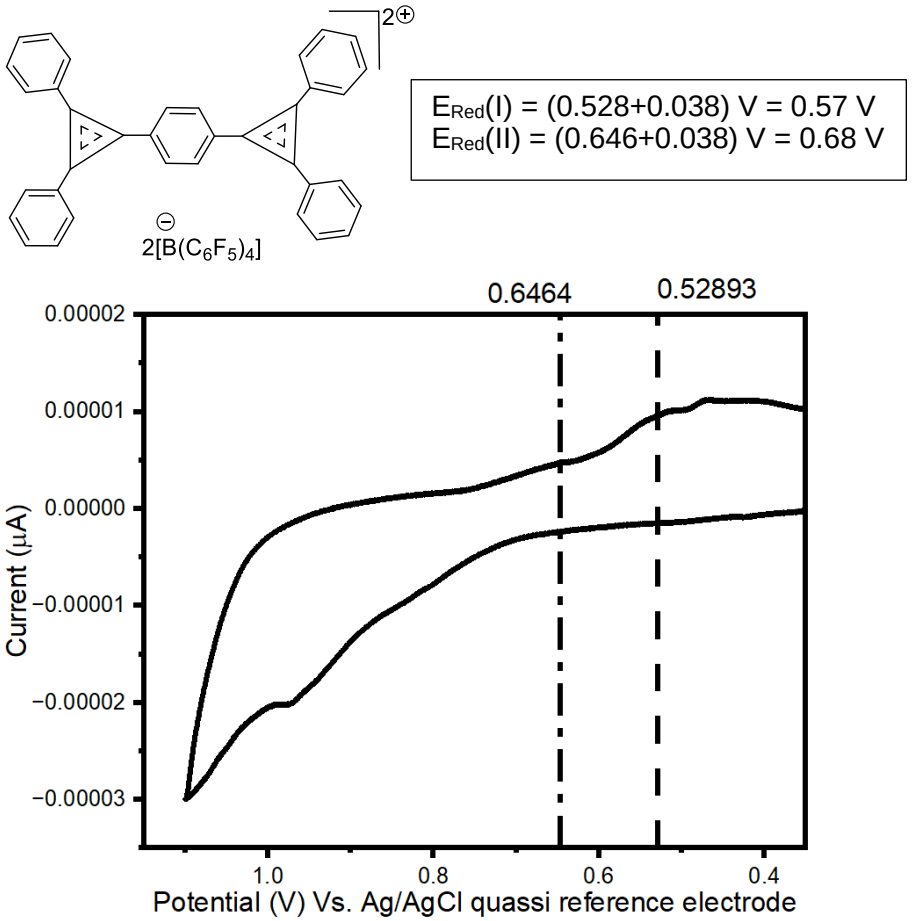


Figure S7. Evolution of CV of **5** (0.1 M) in CH_3CN/DCM (1:1) with $[(n\text{-}Bu)_4N]PF_6$ as supporting electrolyte. Scan rate employed: 0.1 V s^{-1}.

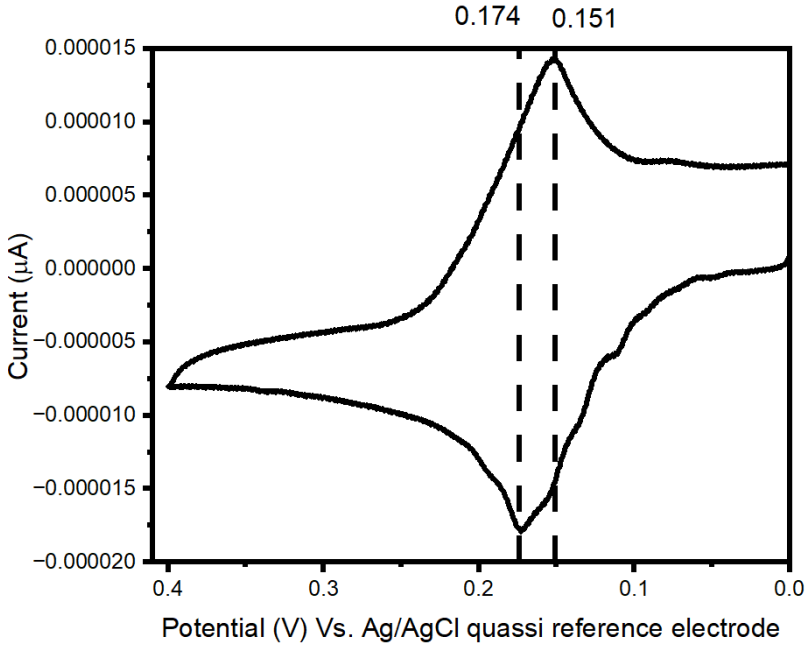
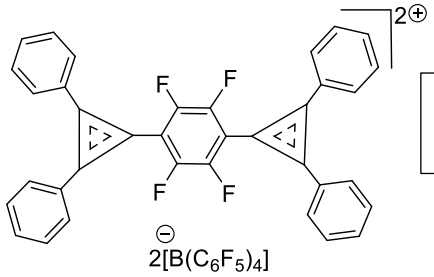


Figure S8. Evolution of CV of **5** with internal ferrocene standard.

Compound 6



E_{Red}(I) = (0.383+0.013) V = 0.40 V
E_{Red}(II) = (0.483+0.013) V = 0.50 V

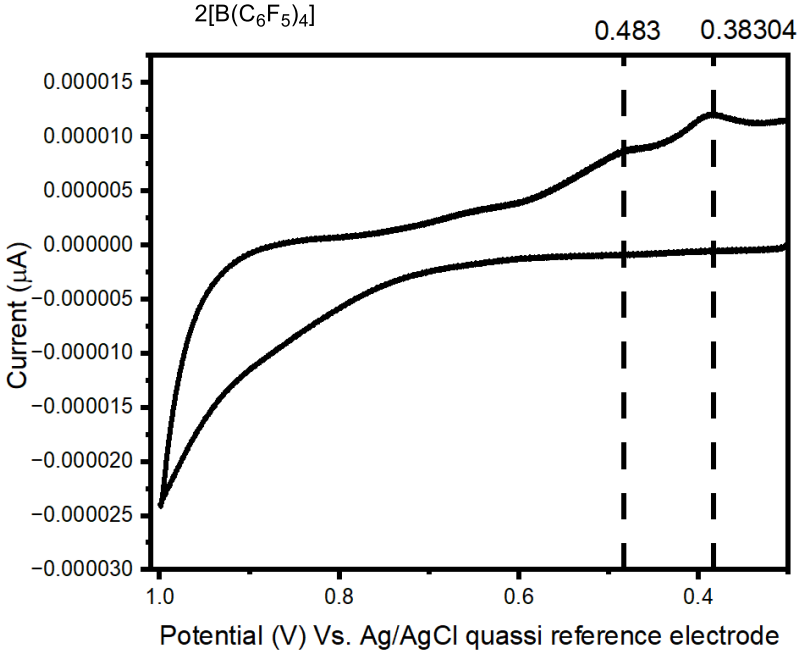


Figure S9. Evolution of CV of **6** (0.1 M) in CH_3CN/DCM (1:1) with [(*n*-Bu)$_4$N]PF_6 as supporting electrolyte. Scan rate employed: 0.1 V s^{-1}.

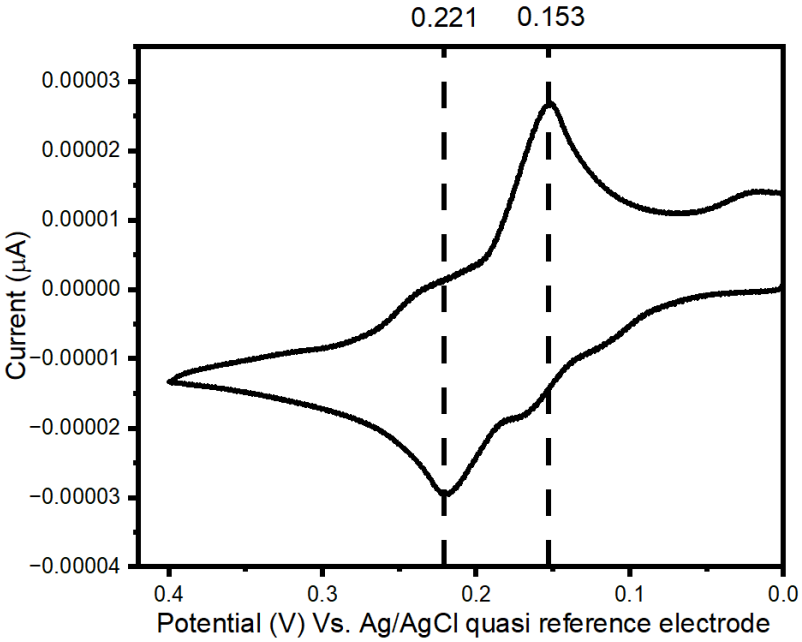
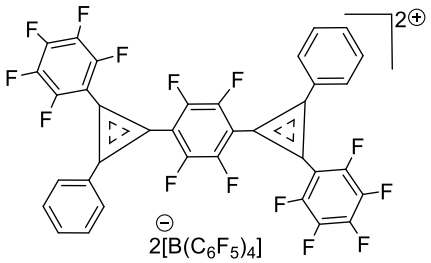


Figure S10. Evolution of CV of **6** with internal ferrocene standard.

Compound 7



E_{Red}(I) = (-0.006+0.061) V = -0.07 V
E_{Red}(II) = (0.193+0.061) V = 0.25 V

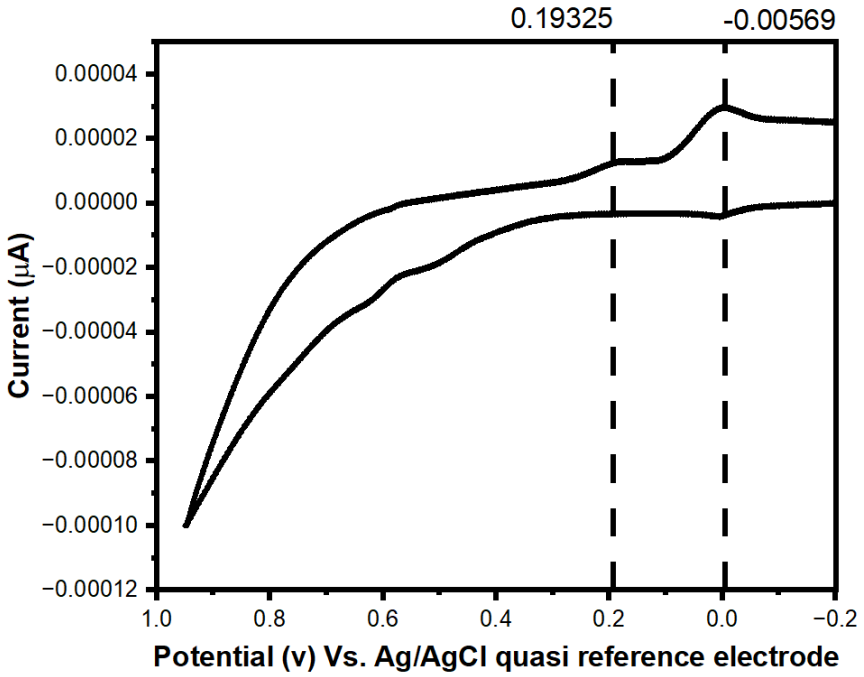


Figure S11. Evolution of CV of **7** (0.1 M) in CH_3CN/DCM (1:1) with $[(n\text{-}Bu)_4N]PF_6$ as supporting electrolyte. Scan rate employed: 0.1 V s^{-1}.

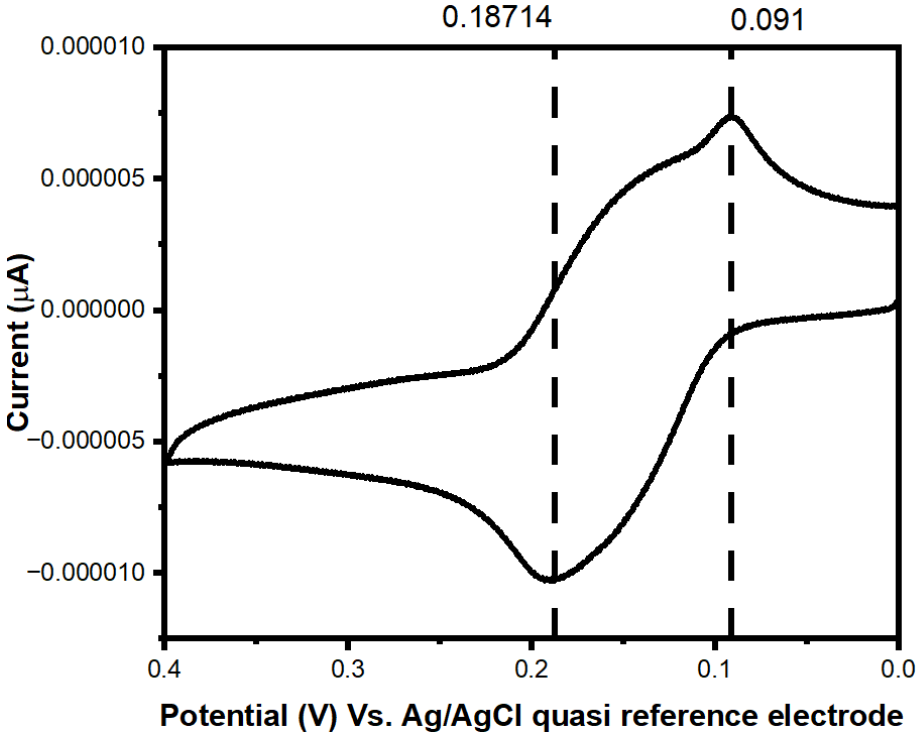


Figure S12. Evolution of CV of **7** with internal ferrocene standard.

NMR spectra of all the compounds

Compound 1

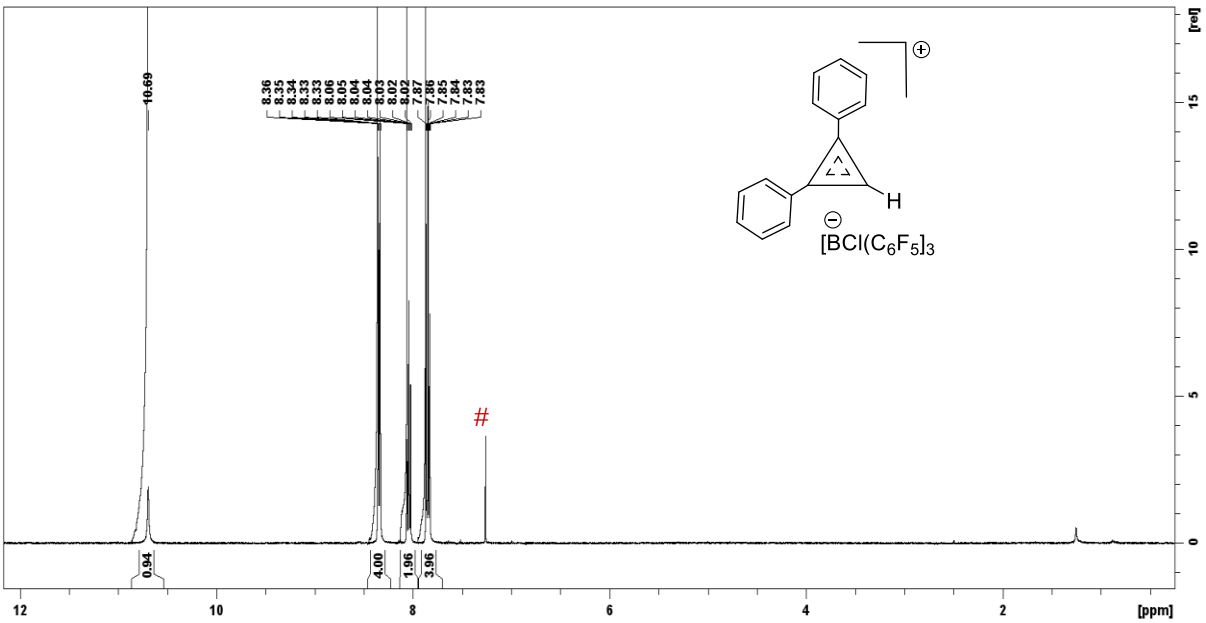


Figure S13. ^{1}H NMR (400 MHz) spectrum of the compound **1** in $CDCl_3$ (#= $CDCl_3$).

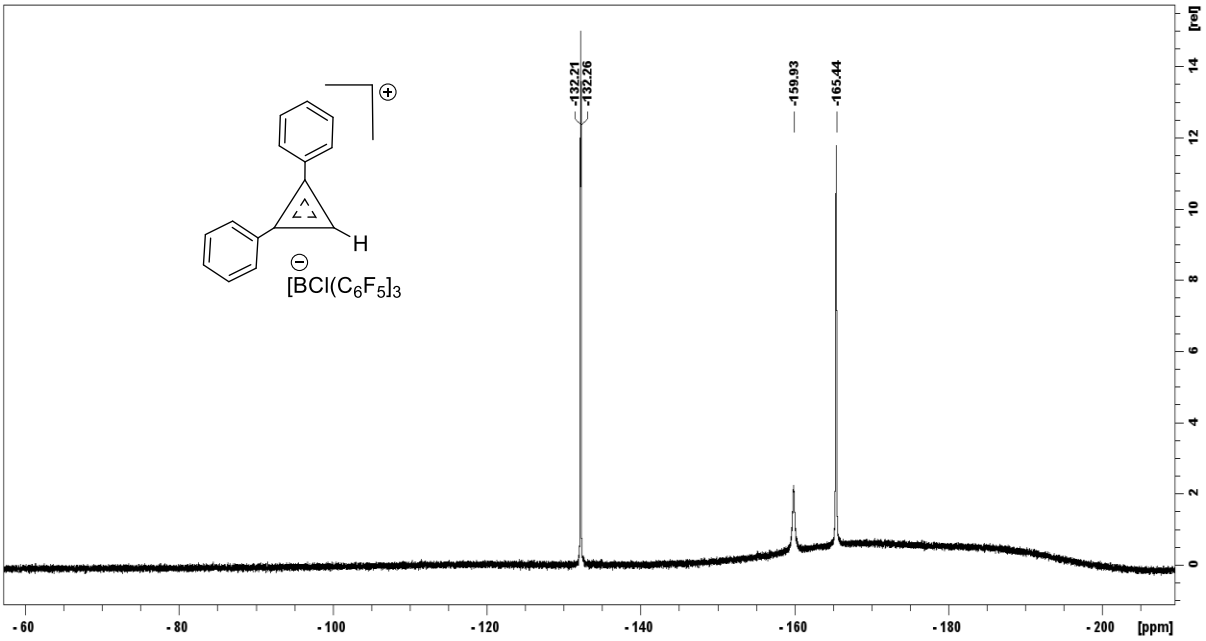


Figure S14. ^{19}F NMR (377 MHz) spectrum of the compound **1** in $CDCl_3$.

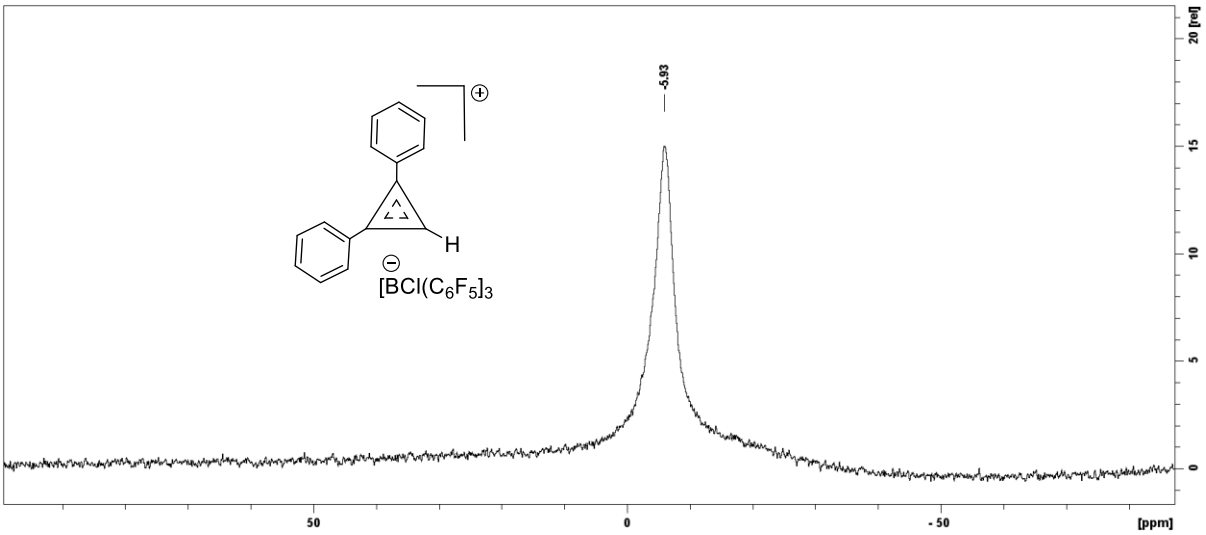


Figure S15. ^{11}B NMR (128 MHz) spectrum of the compound **1** in $CDCl_3$.

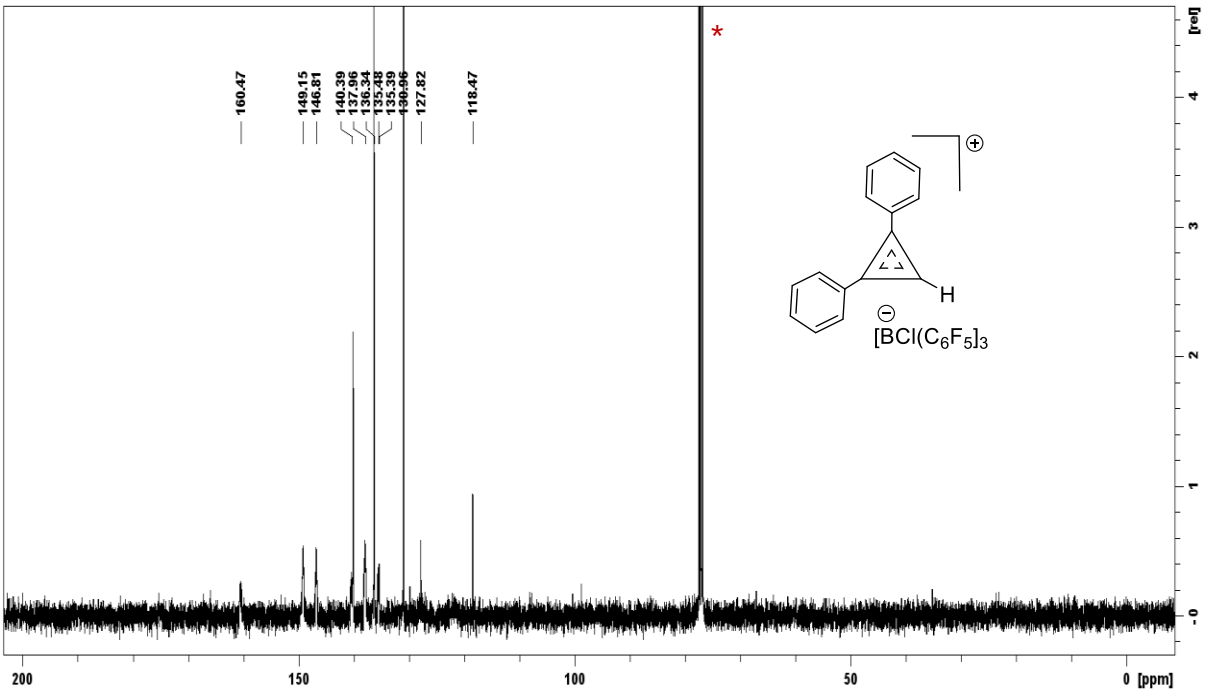


Figure S16. ^{13}C NMR (101 MHz) spectrum of the compound **1** in $CDCl_3$ (*= $CDCl_3$).

Compound 2a

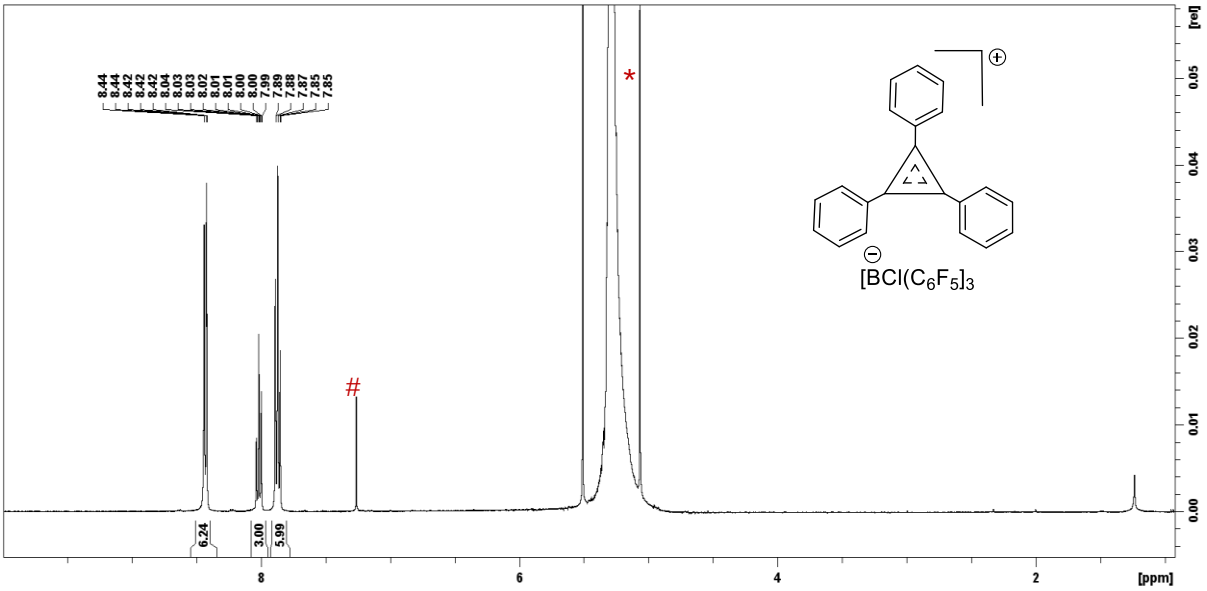


Figure S17. ^{1}H NMR (500 MHz) spectrum of the compound **2a** in $CDCl_3/CH_2Cl_2$ (1:5) (#= $CDCl_3$; *= CH_2Cl_2).

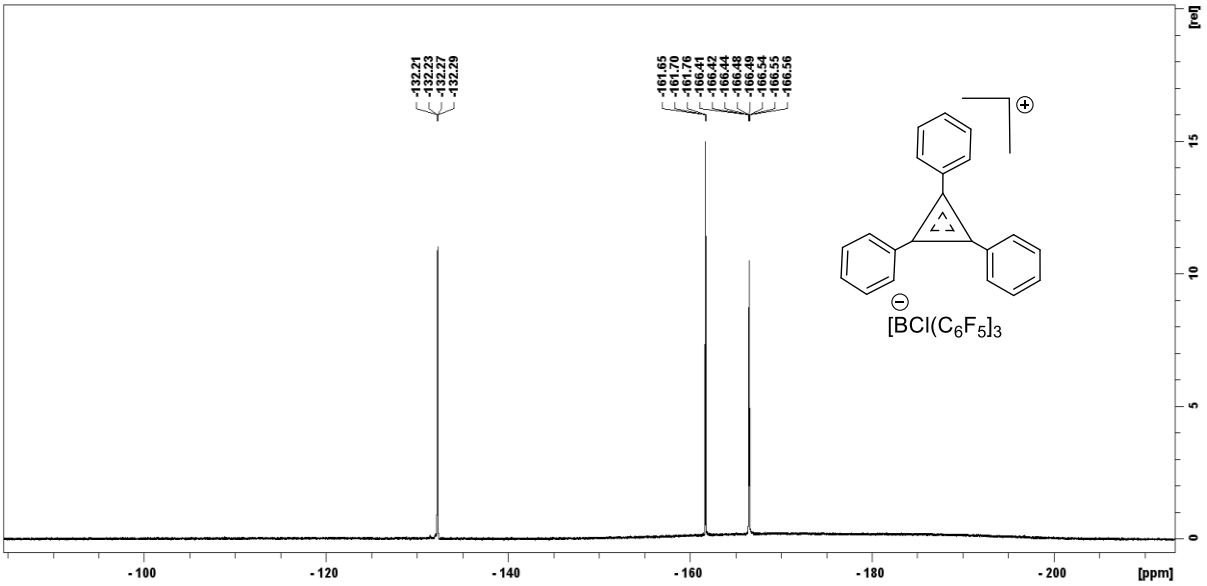


Figure S18. ^{19}F NMR (471 MHz) spectrum of the compound **2a** in $CDCl_3/CH_2Cl_2$ (1:5).

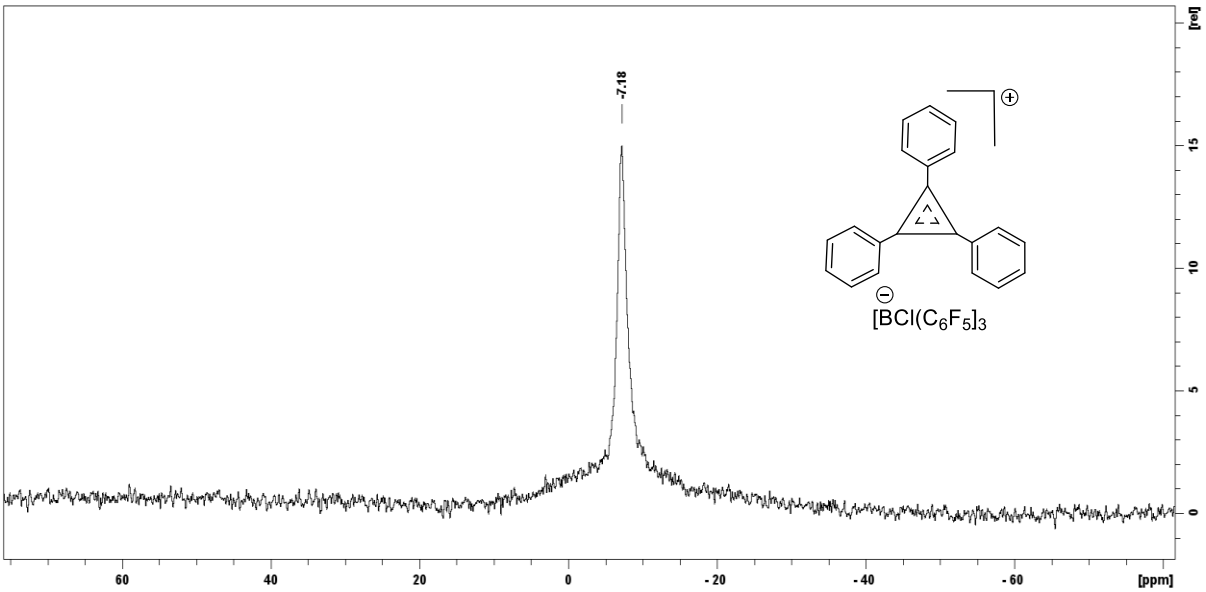


Figure S19. ^{11}B NMR (161 MHz) spectrum of the compound **2a** in $CDCl_3/CH_2Cl_2$ (1:5).

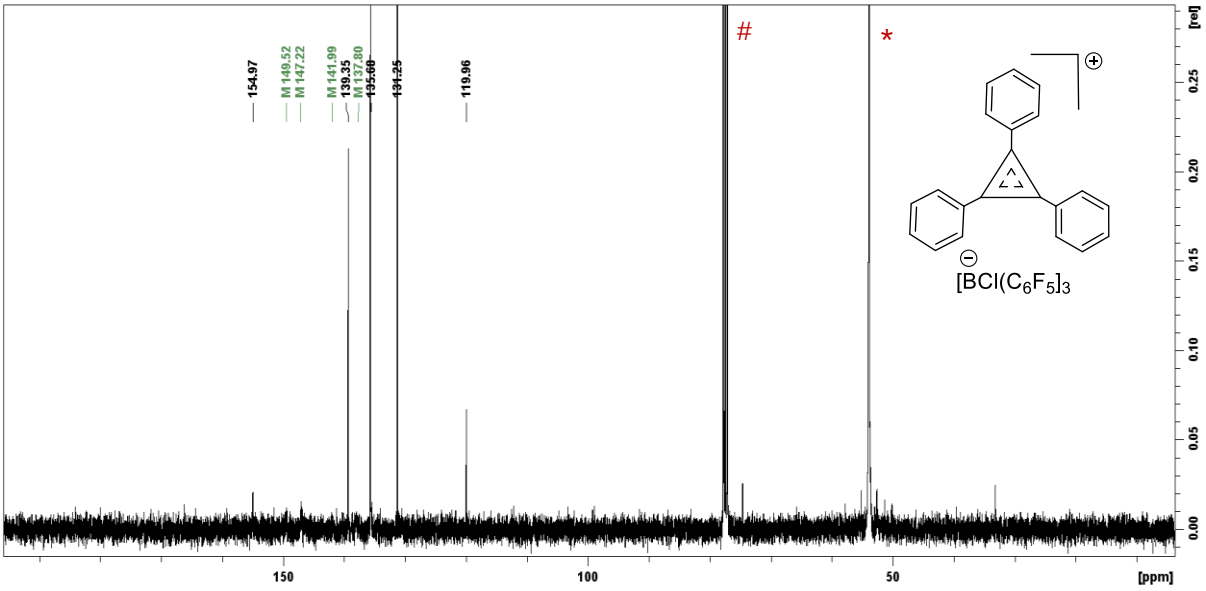


Figure S20. ^{13}C NMR (126 MHz) spectrum of the compound **2a** in $CDCl_3/CH_2Cl_2$ (1:5) (#= $CDCl_3$; *= CH_2Cl_2).

Compound 2b

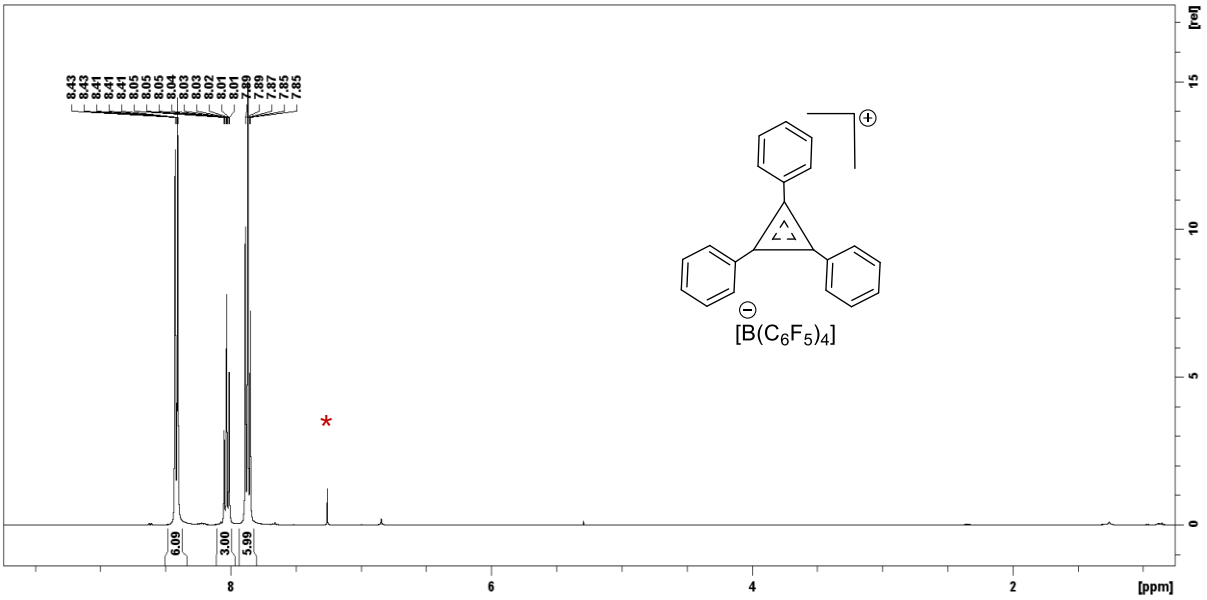


Figure S21. ^{1}H NMR (400 MHz) spectrum of the compound **2b** in $CDCl_3$ (*= $CDCl_3$).

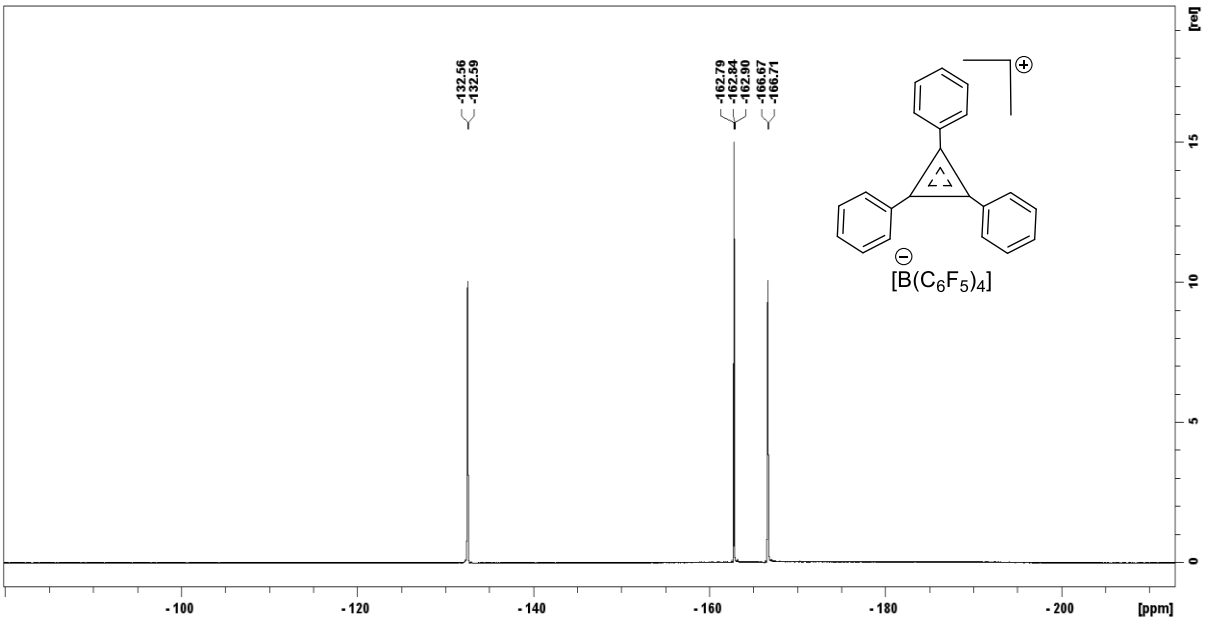


Figure S22. ^{19}F NMR (377 MHz) spectrum of the compound **2b** in $CDCl_3$.

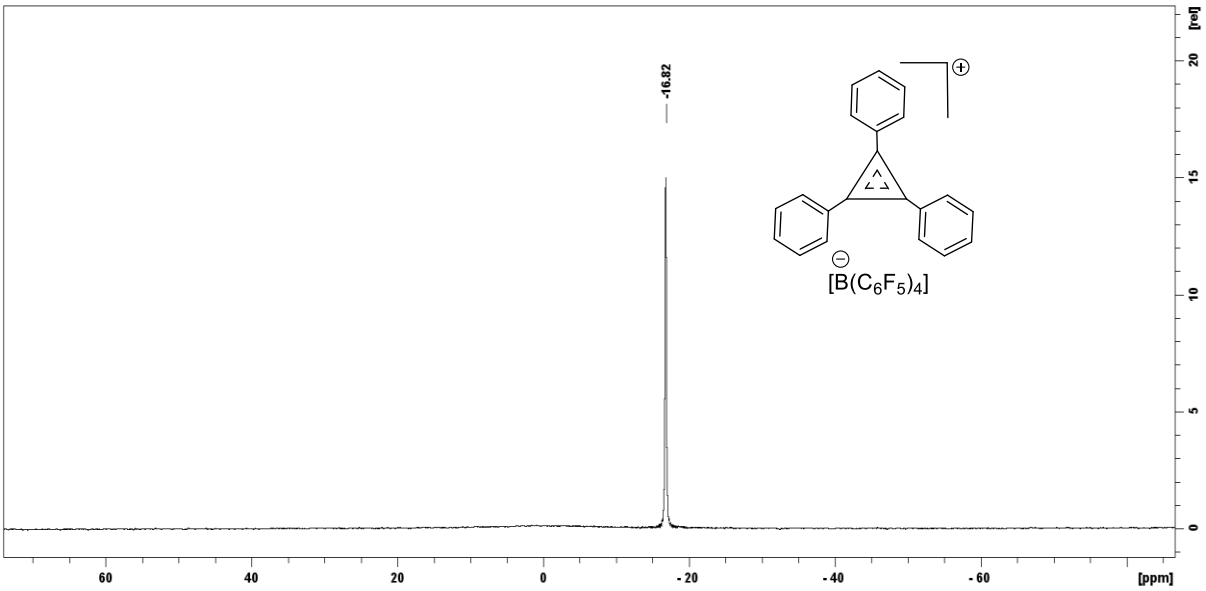


Figure S23. ^{11}B NMR (128 MHz) spectrum of the compound **2b** in $CDCl_3$.

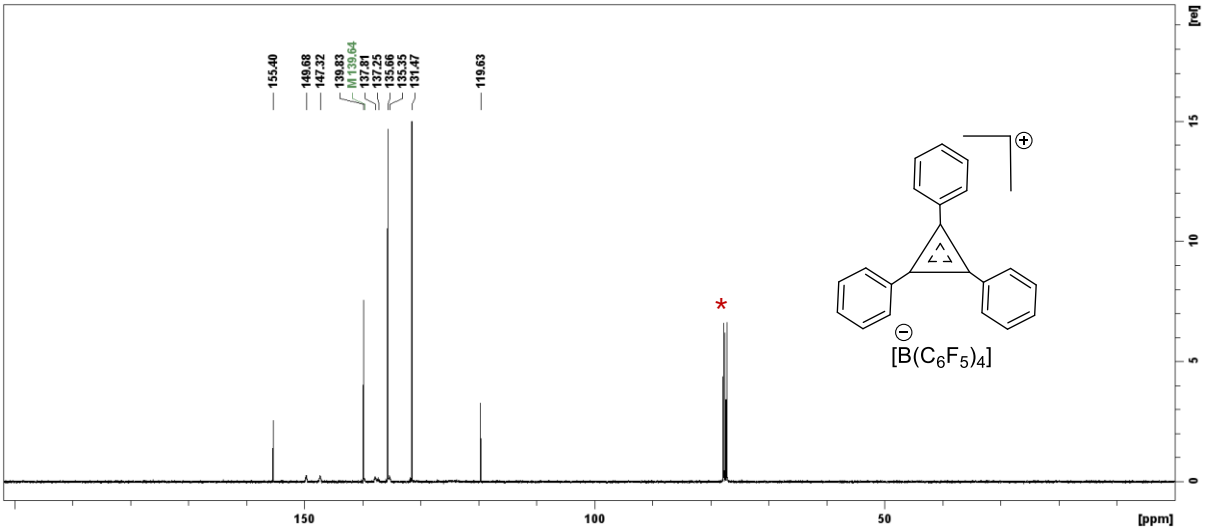


Figure S24. ^{13}C NMR (101 MHz) spectrum of the compound **2b** in $CDCl_3$ (*= $CDCl_3$).

Compound 2c

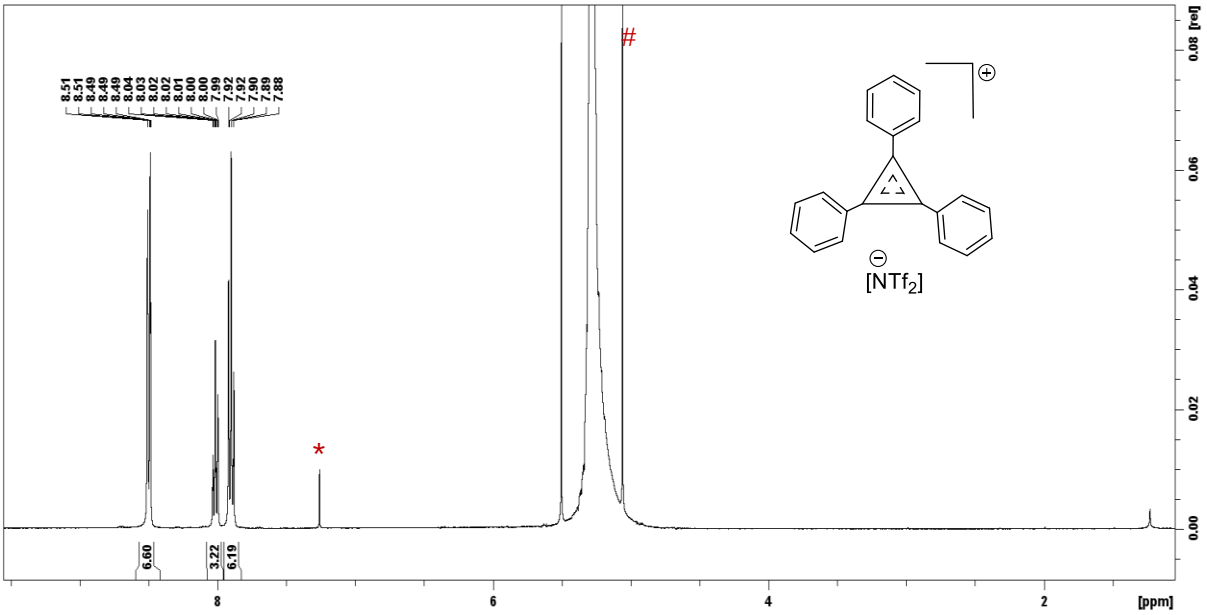


Figure S25. 1H NMR (400 MHz) spectrum of the compound **2c** in $CDCl_3/CH_2Cl_2$ (1:5) (*= $CDCl_3$; #= CH_2Cl_2).

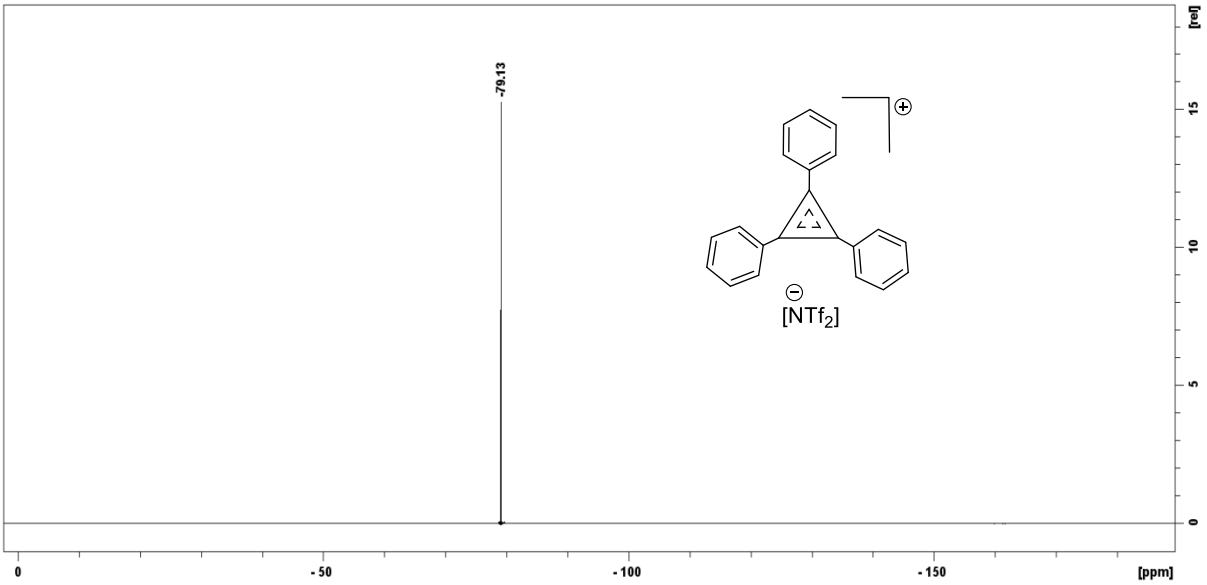


Figure S26. ^{19}F NMR (377 MHz) spectrum of the compound **2c** in $CDCl_3/CH_2Cl_2$ (1:5).

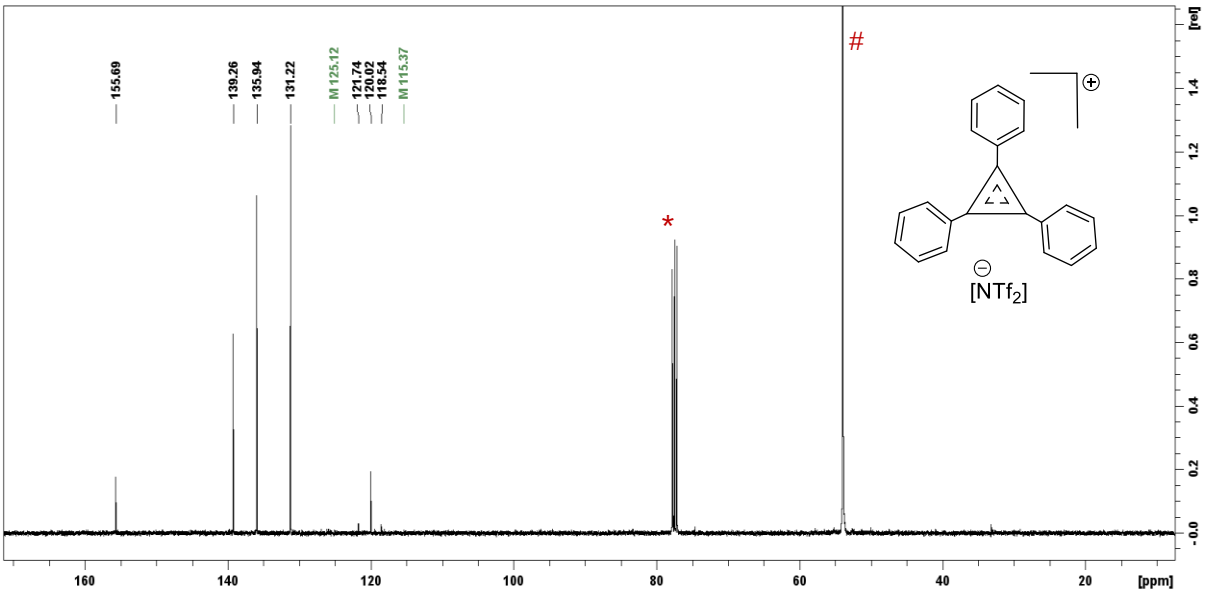


Figure S27. ^{13}C NMR (101 MHz) spectrum of the compound **2c** in $CDCl_3/CH_2Cl_2$ (1:5) (*= $CDCl_3$; #= CH_2Cl_2).

Compound 3

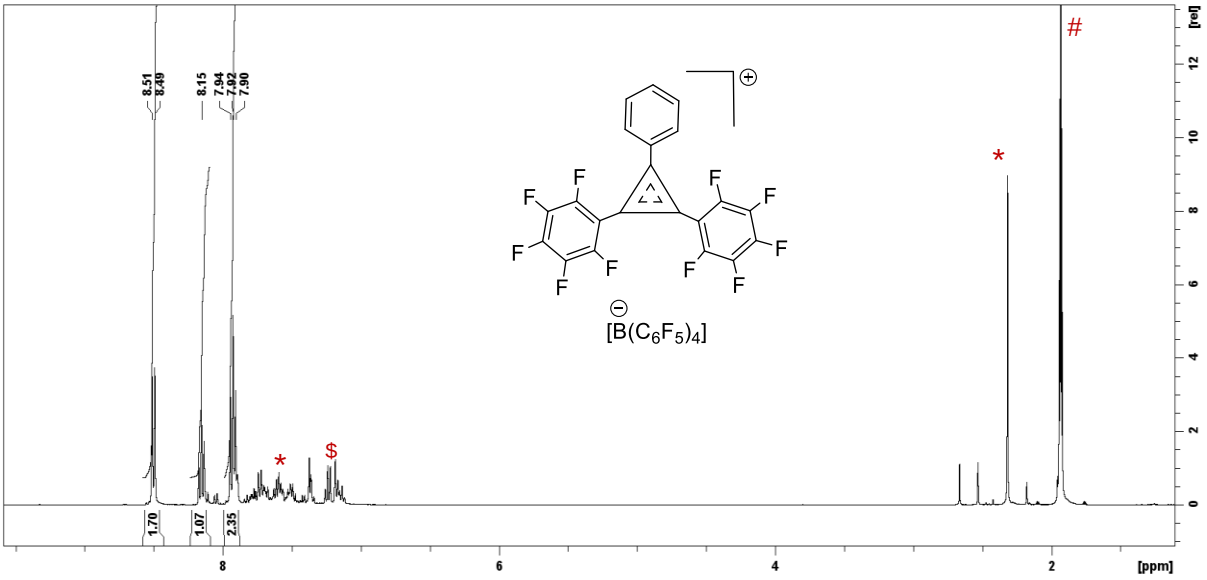


Figure S28. 1H NMR (400 MHz) spectrum of the compound **3** in CD_3CN (*= residual toluene; $= unidentified impurities; #= CD_3CN).

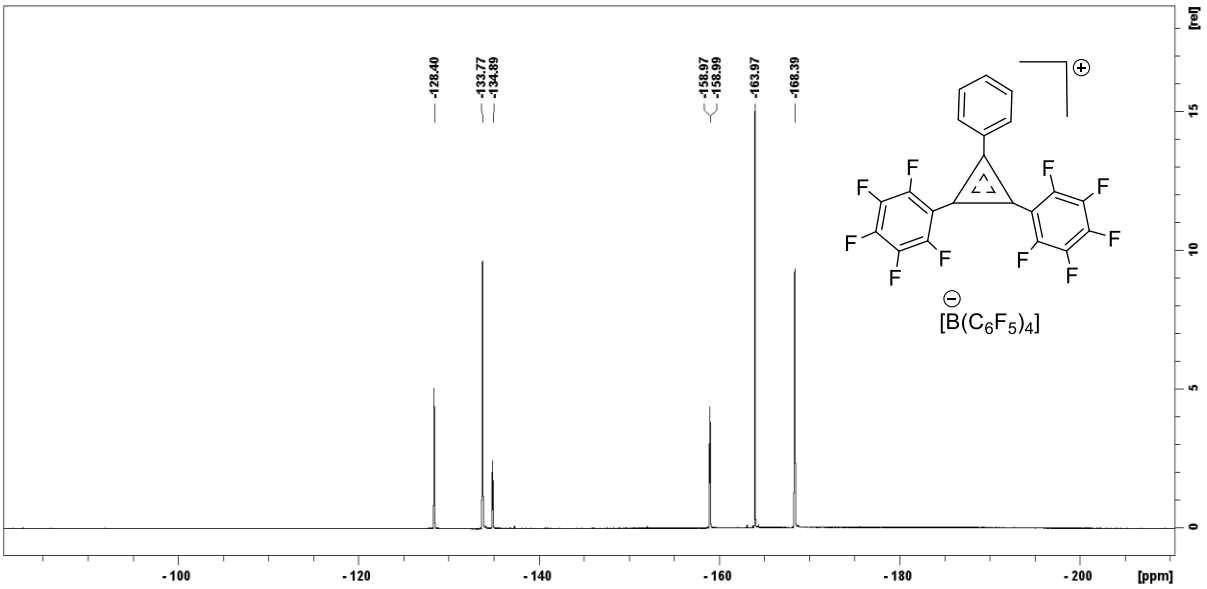


Figure S29. ^{19}F NMR (377 MHz) spectrum of the compound **3** in CD_3CN.

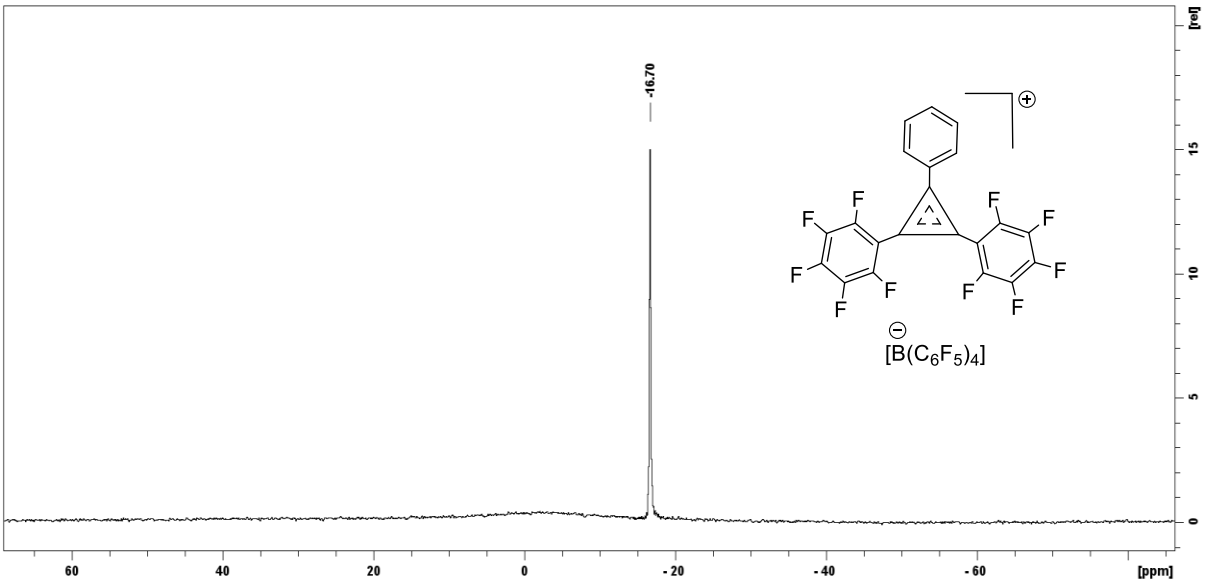


Figure S30. ^{11}B NMR (128 MHz) spectrum of the compound **3** in CD_3CN.

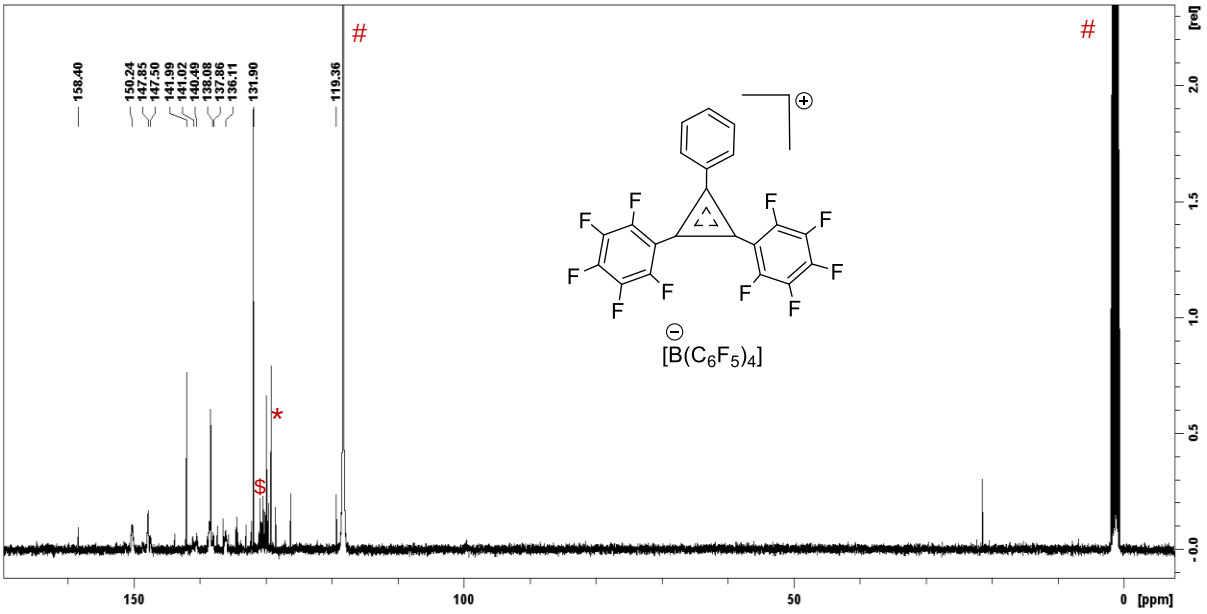


Figure S31. ^{13}C NMR (101 MHz) spectrum of the compound **3** in CD_3CN (*= residual toluene; $= unidentified impurities; #= CD_3CN).

Compound 4a

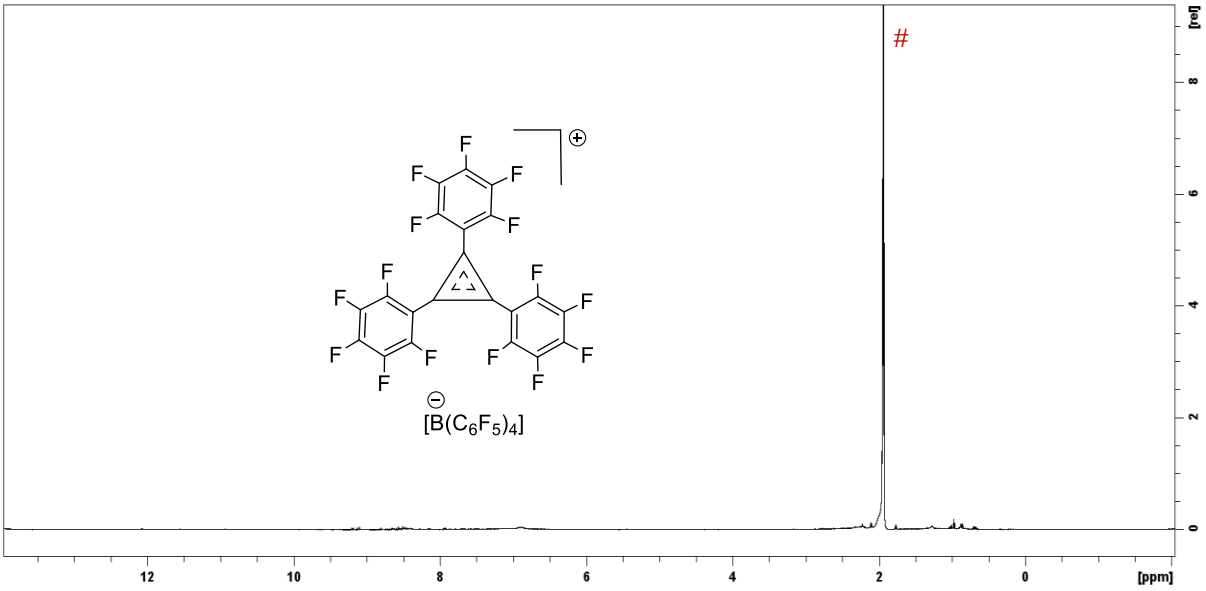


Figure S32. ^{1}H NMR (400 MHz) spectrum of the compound **4a** in CD_3CN (#= CD_3CN).

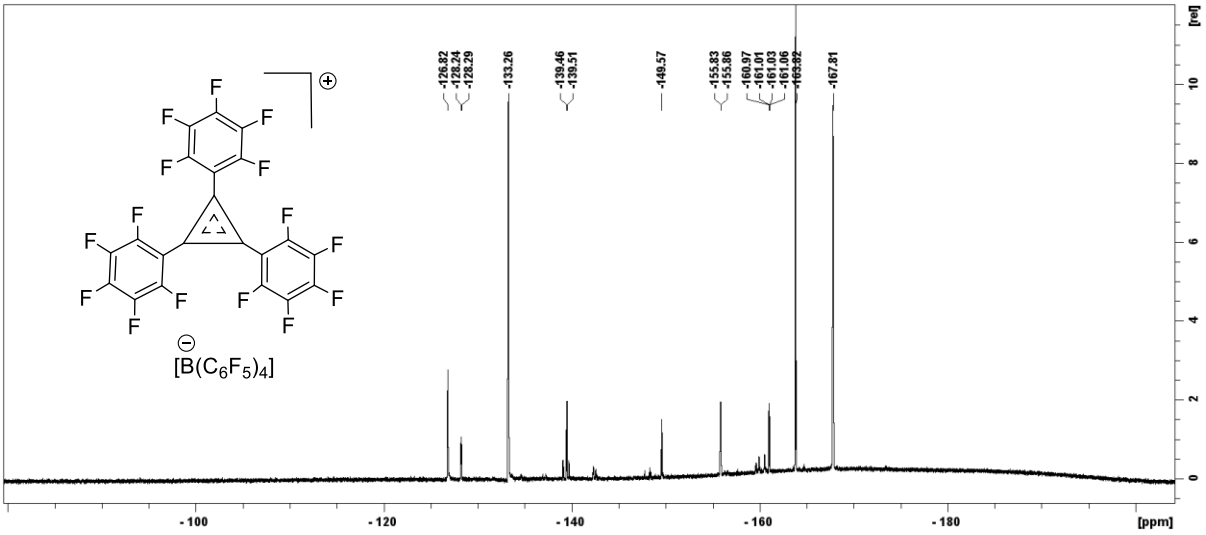


Figure S33. ^{19}F NMR (377 MHz) spectrum of the compound **4a** in CD_3CN.

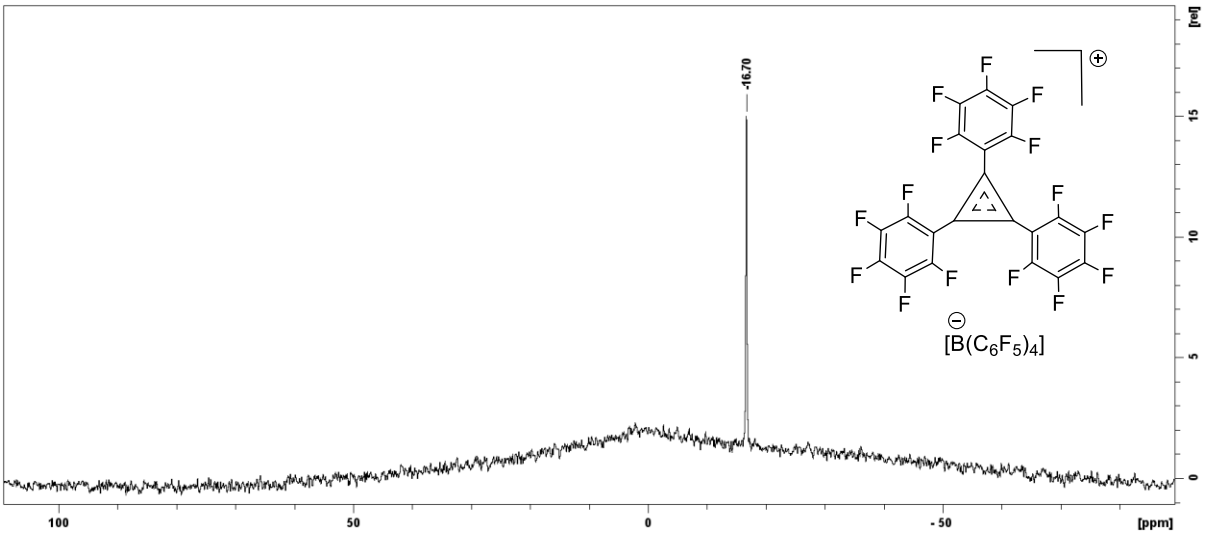


Figure S34. ^{11}B NMR (128 MHz) spectrum of the compound **4a** in CD_3CN.

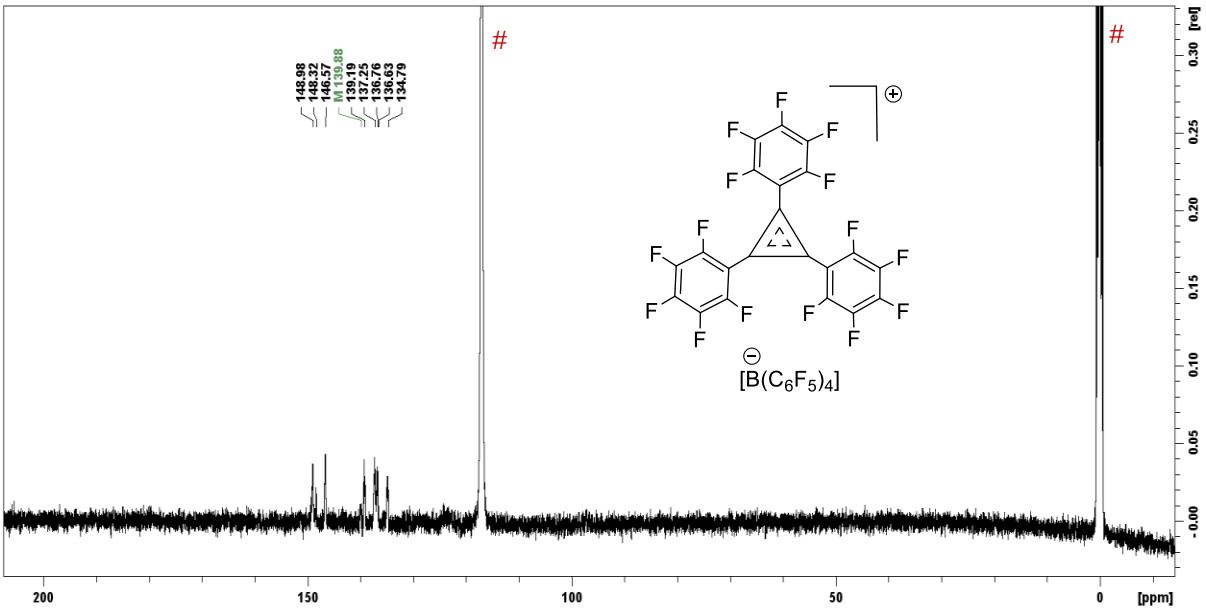


Figure S35. ^{13}C NMR (101 MHz) spectrum of the compound **4a** in CD_3CN (#= CD_3CN).

Compound 4b

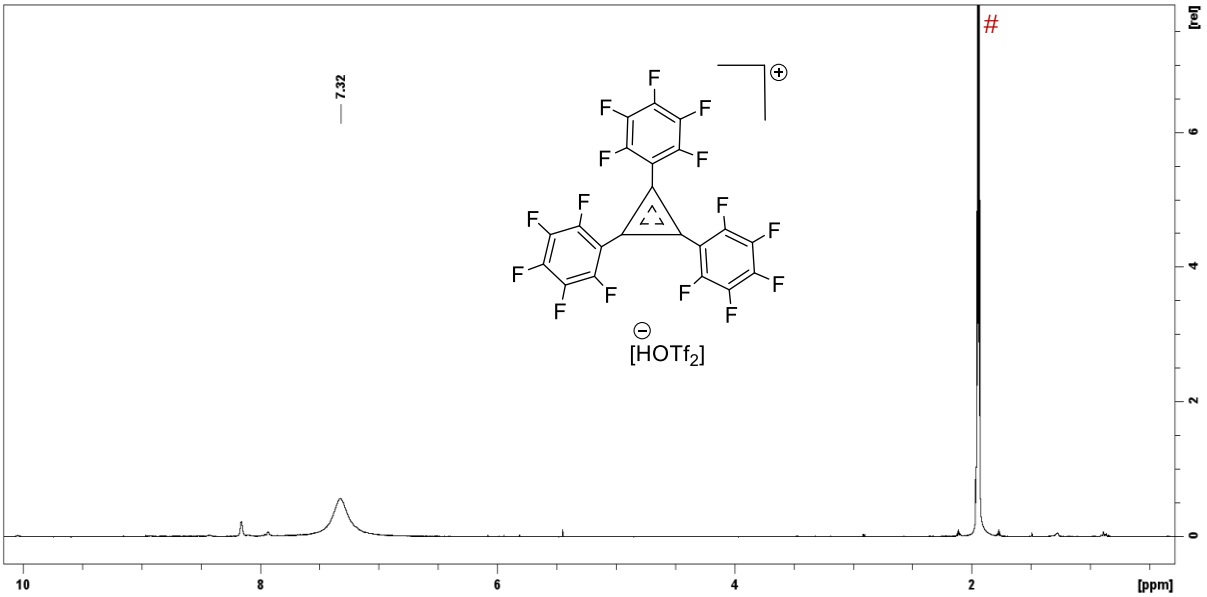


Figure S36. ^{1}H NMR (400 MHz) spectrum of the compound **4b** in CD_3CN (#= CD_3CN).

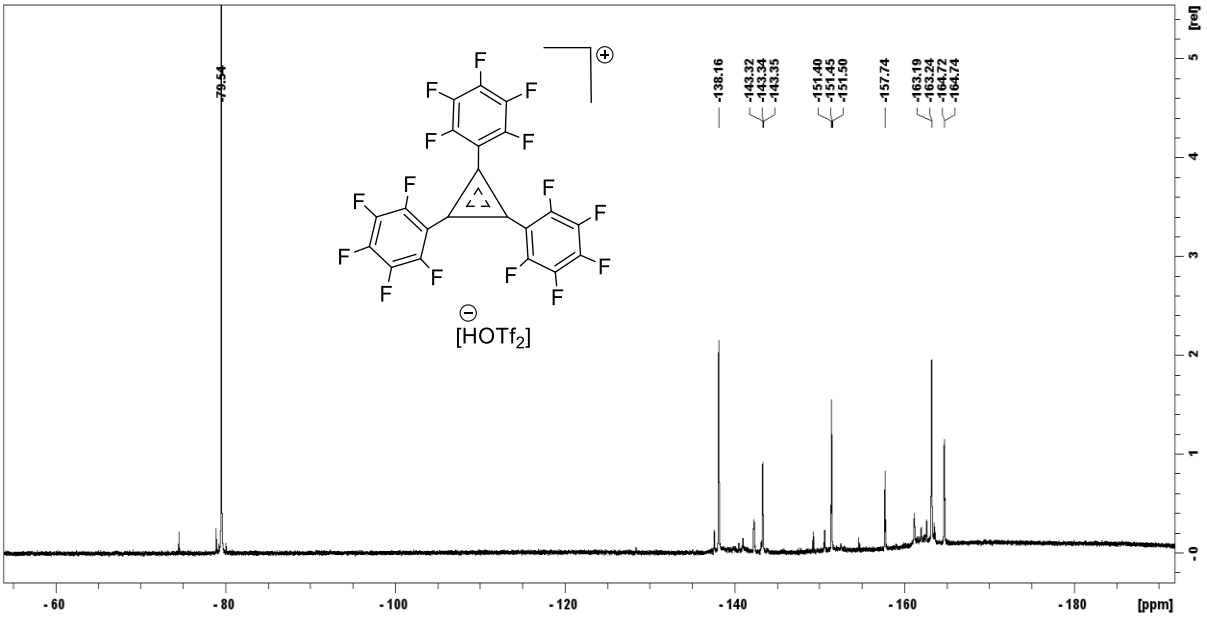


Figure S37. ^{19}F NMR (377 MHz) spectrum of the compound **4b** in CD_3CN.

Compound 5

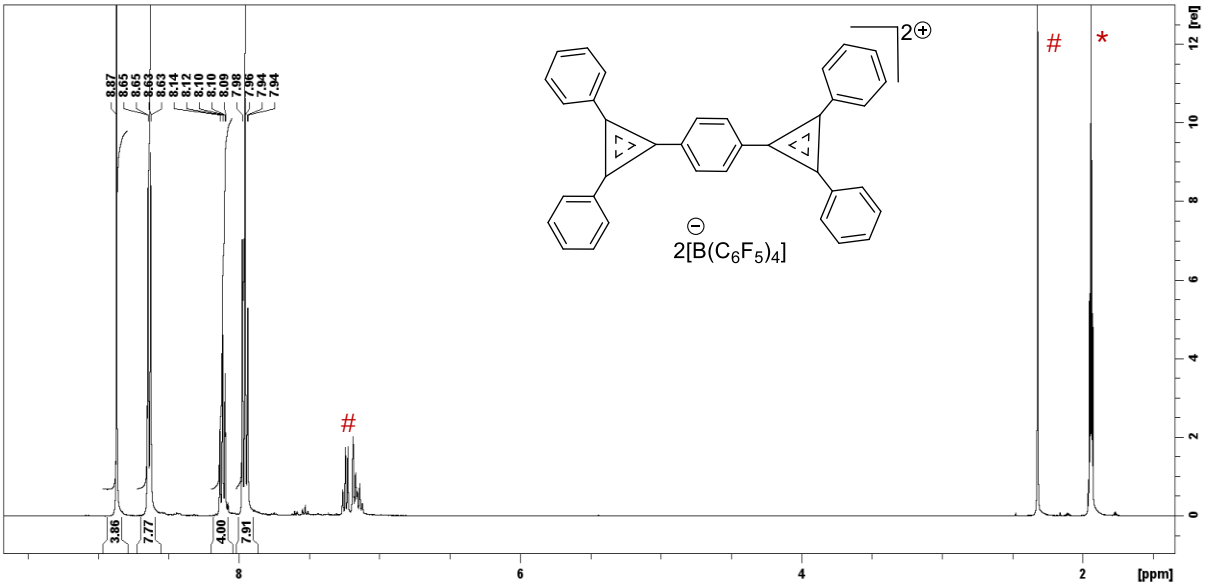


Figure S38. ^{1}H NMR (400 MHz) spectrum of the compound **5** in CD_3CN (*= CD_3CN, #= residual toluene).

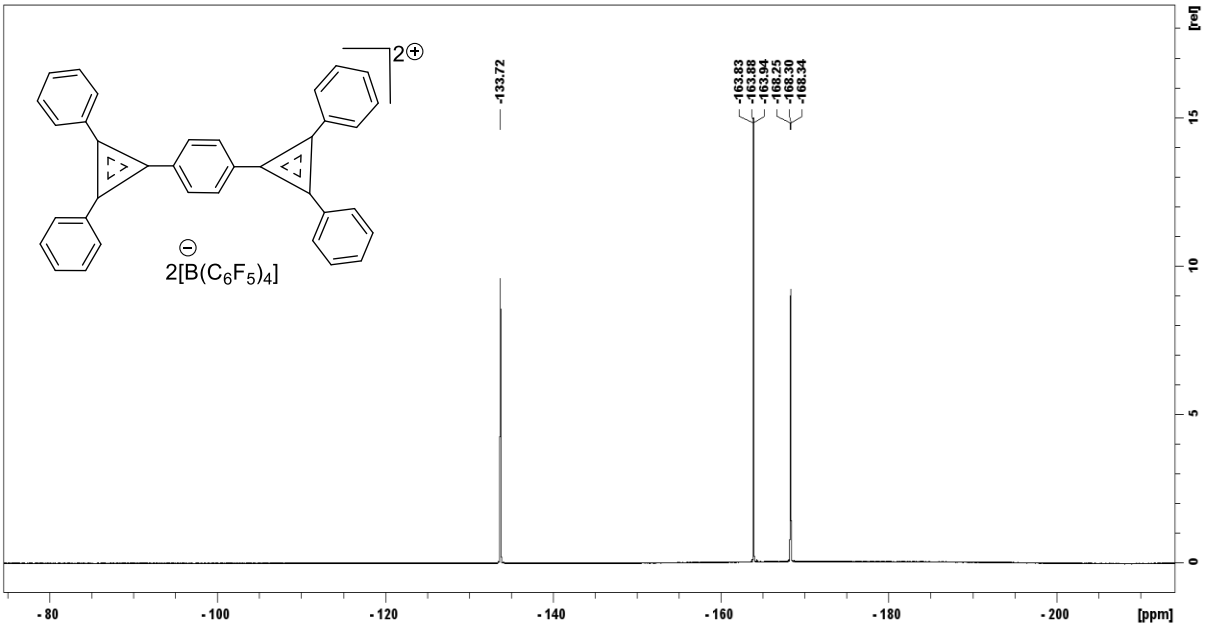


Figure S39. ^{19}F NMR (377 MHz) spectrum of the compound **5** in CD_3CN.

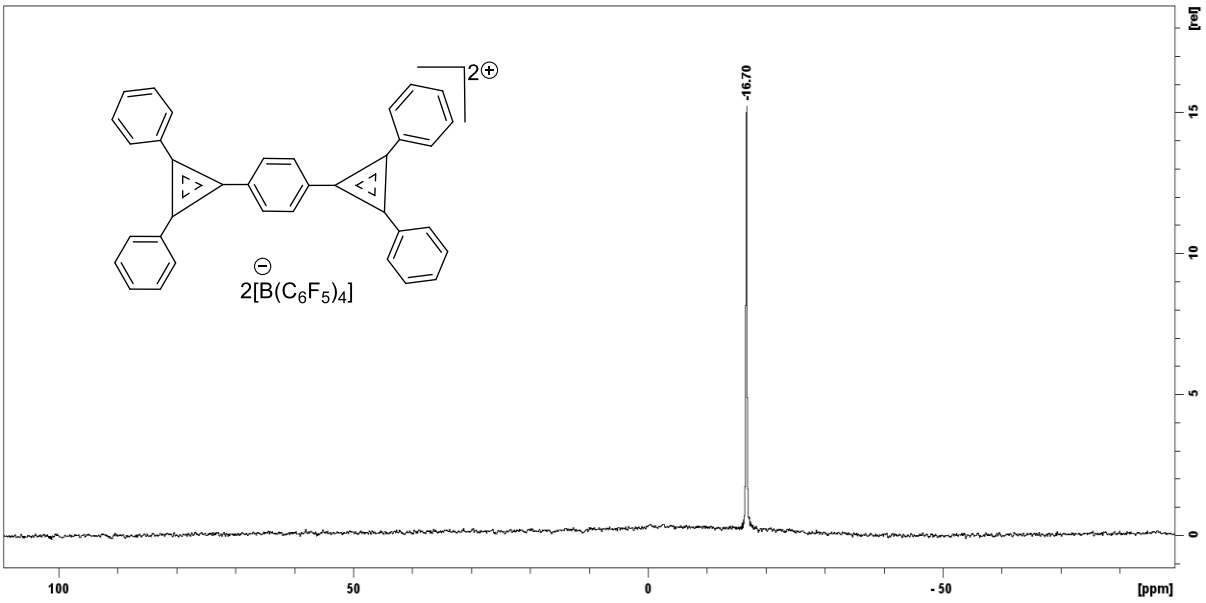


Figure S40. ^{11}B NMR (128 MHz) spectrum of the compound **5** in CD_3CN.

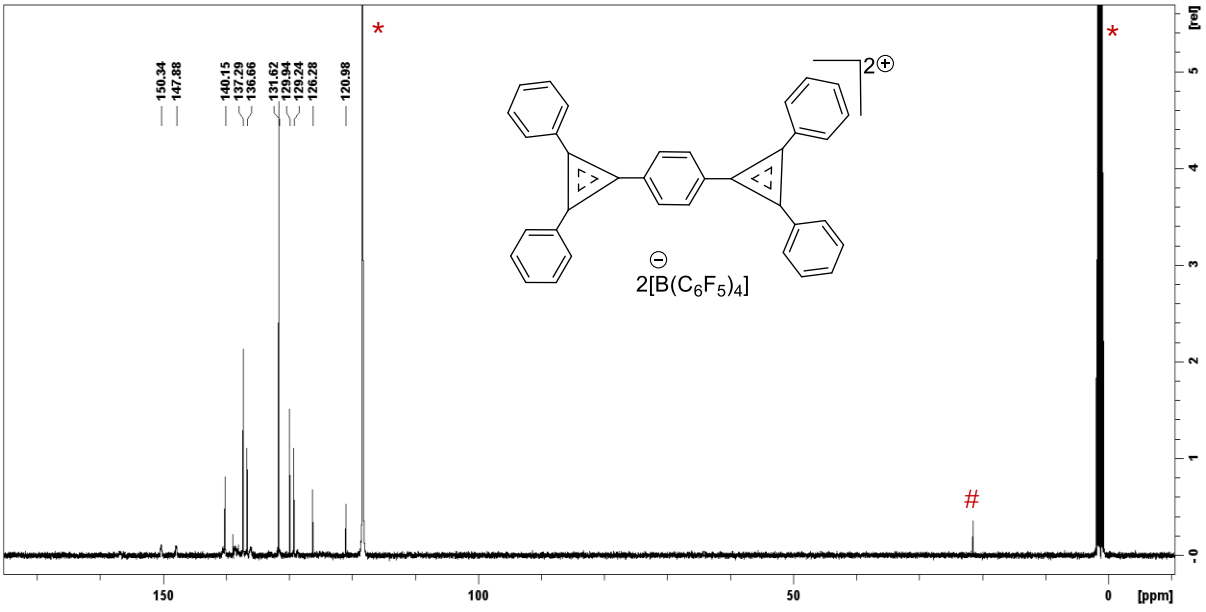


Figure S41. ^{13}C NMR (101 MHz) spectrum of the compound **5** in CD_3CN (*= CD_3CN, #= residual toluene).

Compound 6

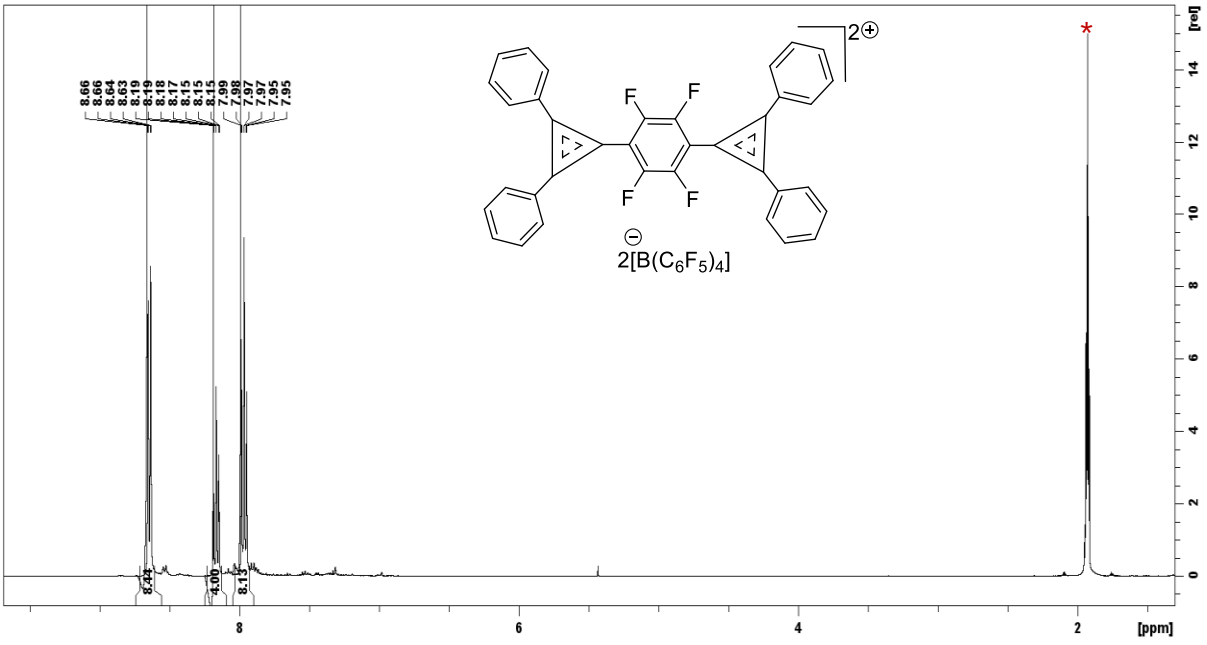


Figure S42. ^{1}H NMR (500 MHz) spectrum of the compound **6** in CD_3CN (*= CD_3CN).

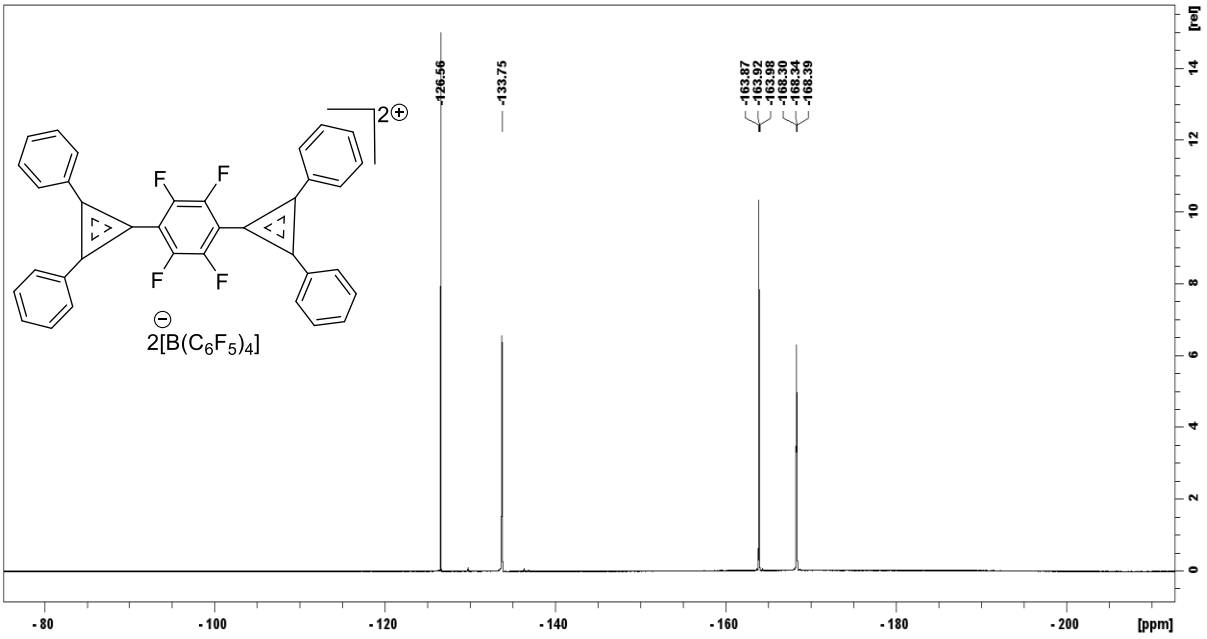


Figure S43. ^{19}F NMR (377 MHz) spectrum of the compound **6** in CD_3CN.

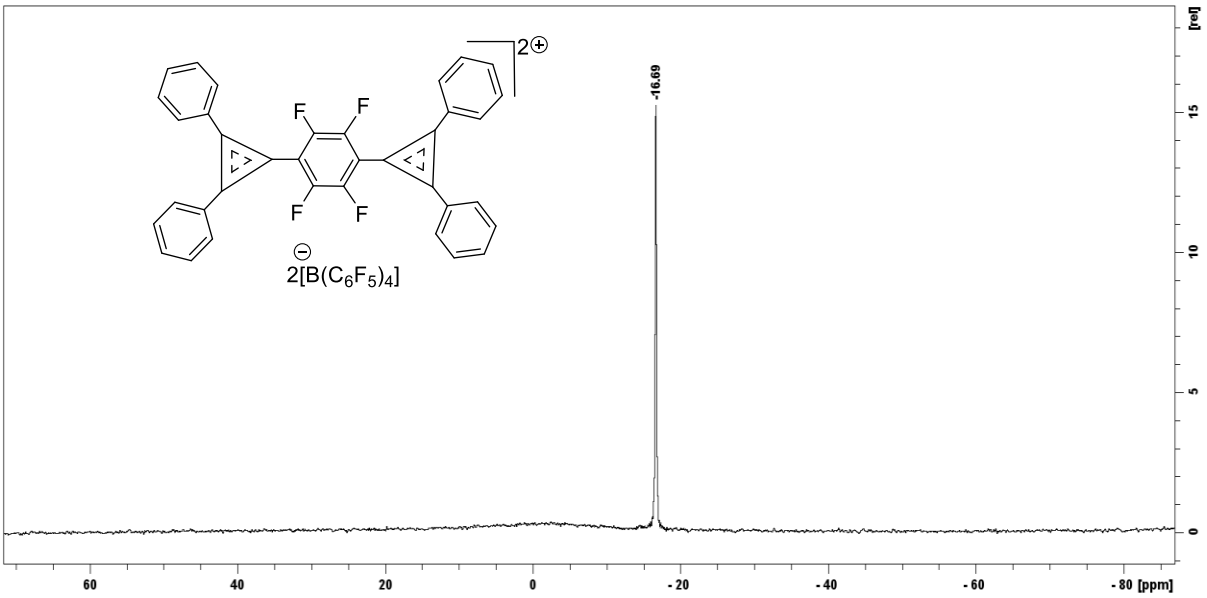


Figure S44. ^{11}B NMR (161 MHz) spectrum of the compound **6** in CD_3CN.

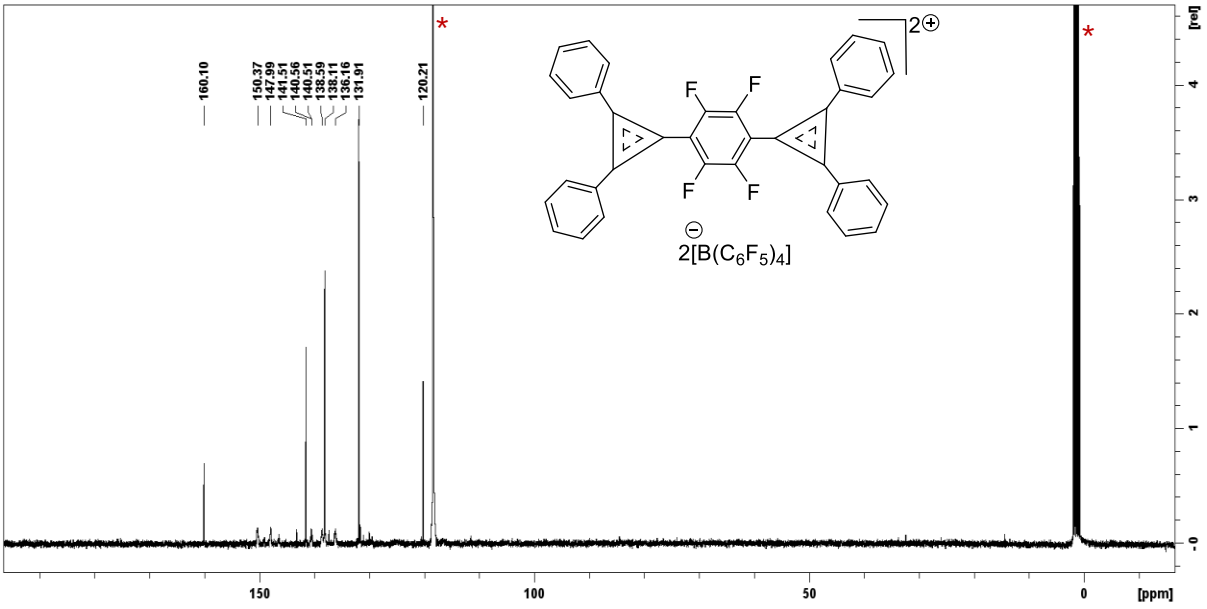


Figure S45. ^{13}C NMR (101 MHz) spectrum of the compound **6** in CD_3CN (*= CD_3CN).

Compound 7

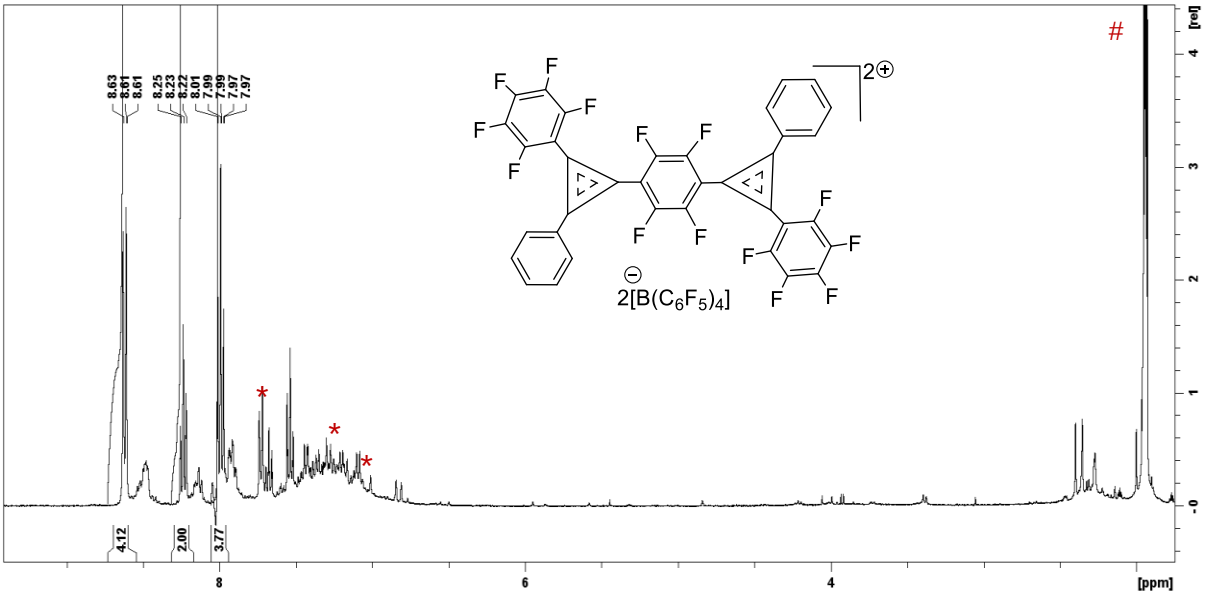


Figure S46. ^{1}H NMR (400 MHz) spectrum of the compound **7** in CD_3CN (*= unidentified impurities; #= CD_3CN).

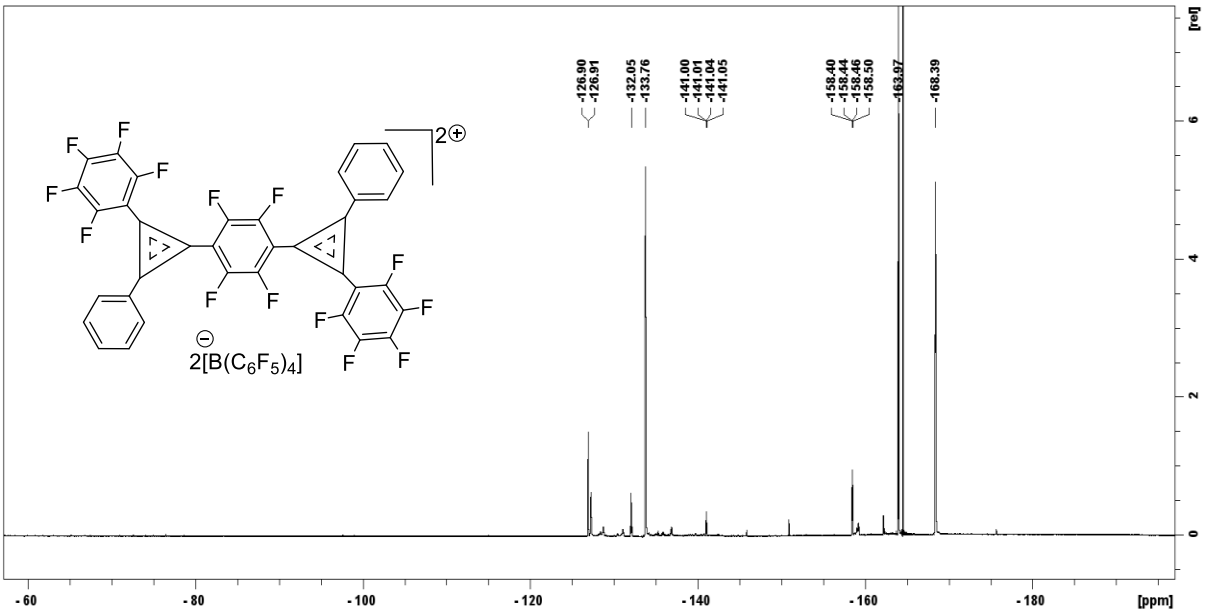


Figure S47. ^{19}F NMR (377 MHz) spectrum of the compound **7** in CD_3CN.

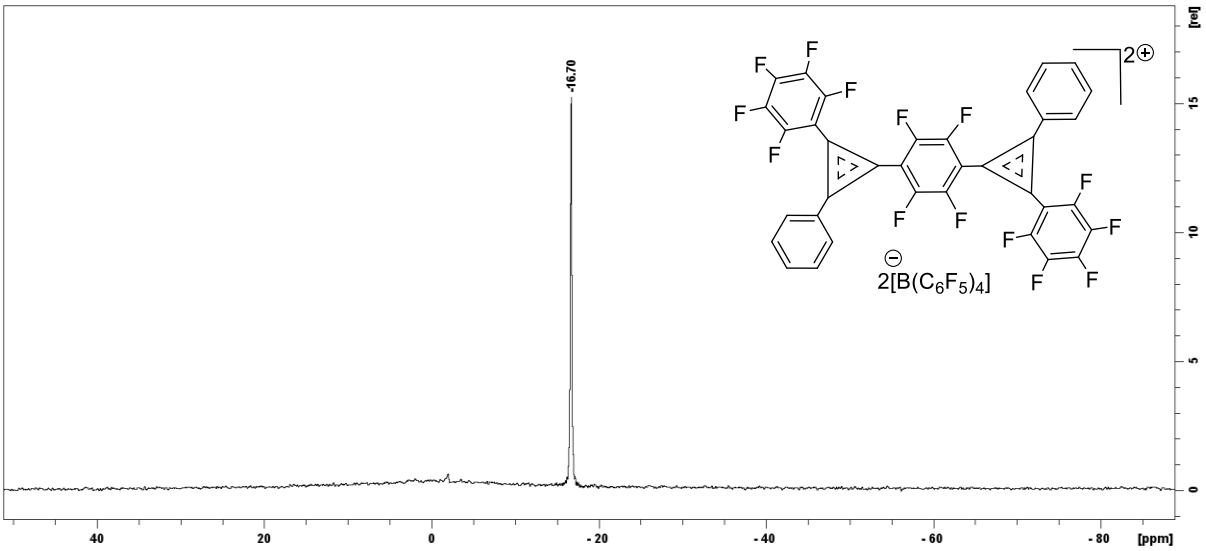


Figure S48. ^{11}B NMR (128 MHz) spectrum of the compound **7** in CD_3CN.

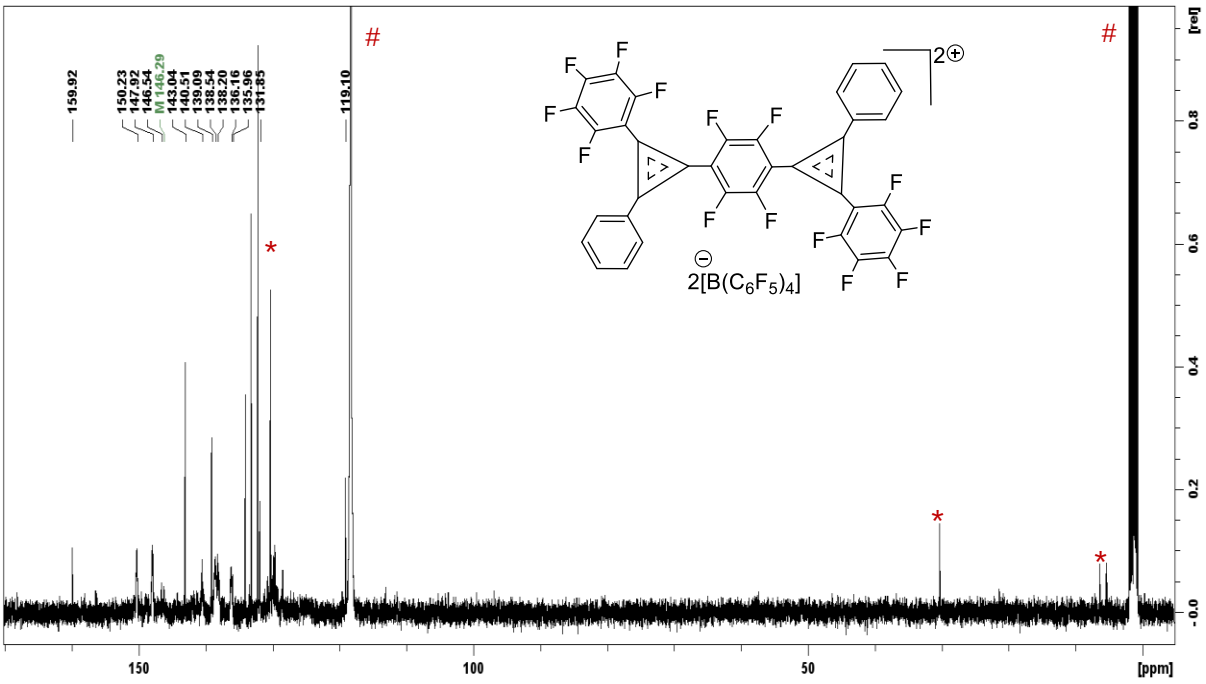


Figure S49. ^{13}C NMR (101 MHz) spectrum of the compound **7** in CD_3CN (*= unidentified impurities, #= CD_3CN).

Compound 8

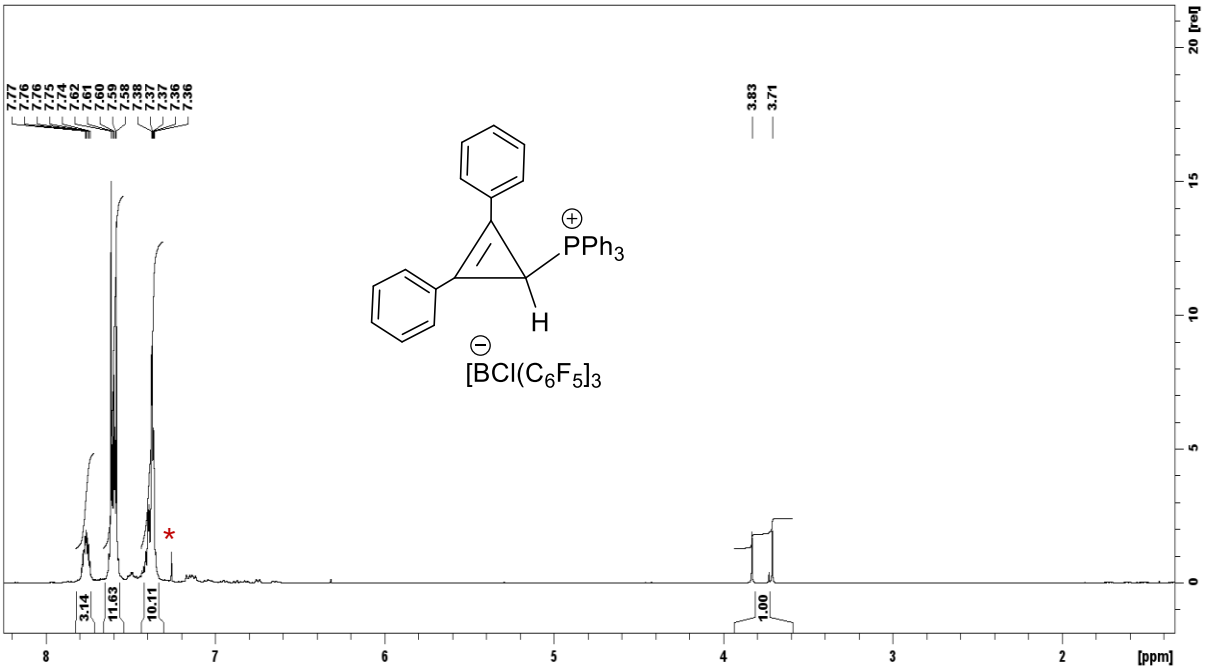


Figure S50. ^{1}H NMR (400 MHz) spectrum of the compound **8** in $CDCl_3$ (*= $CDCl_3$).

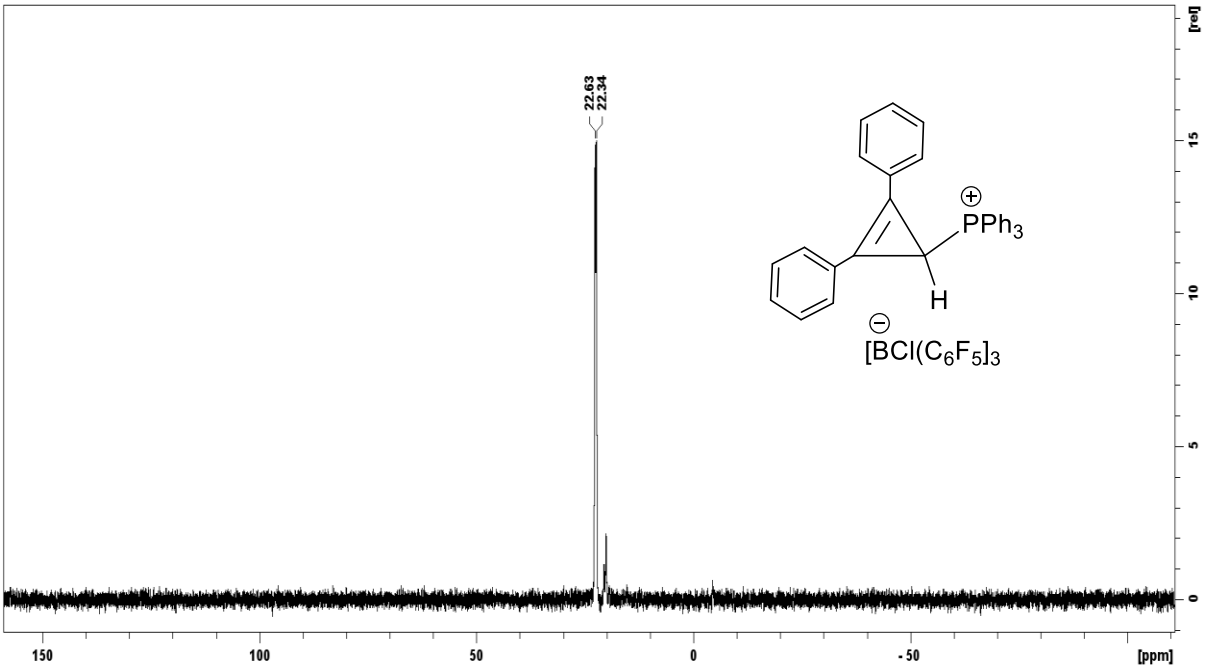


Figure S51. ^{31}P NMR (162 MHz) spectrum of the compound **8** in $CDCl_3$.

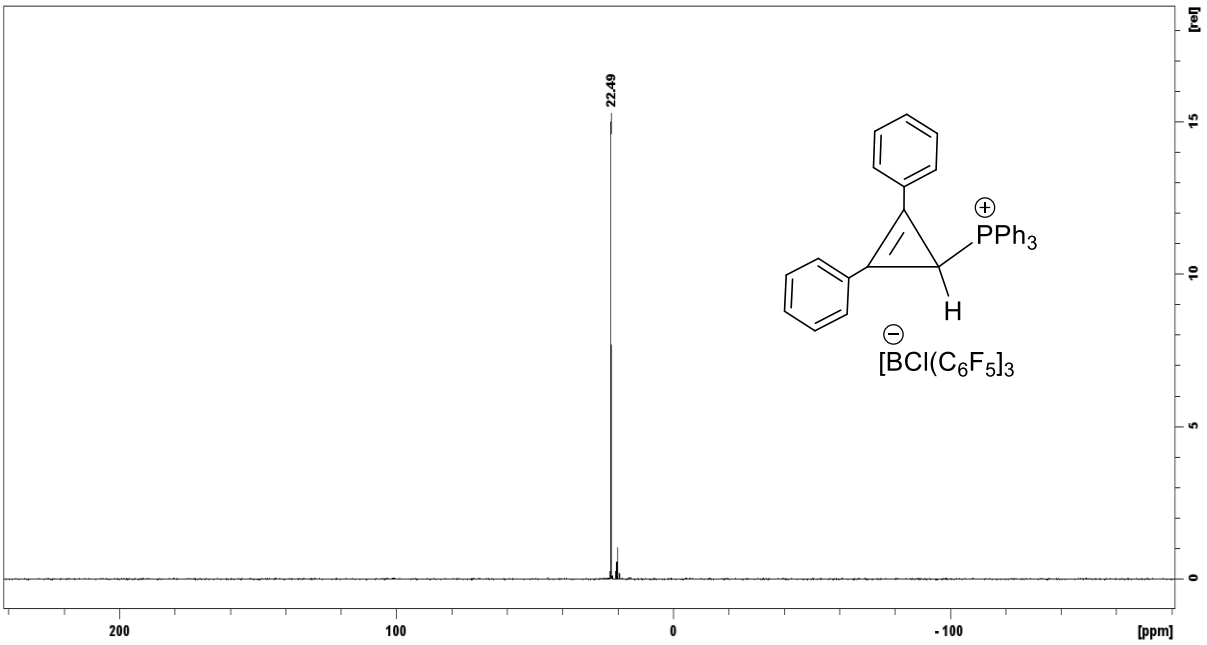


Figure S52. $^{31}P\{^{1}H\}$ NMR (162 MHz) spectrum of the compound **8** in $CDCl_3$.

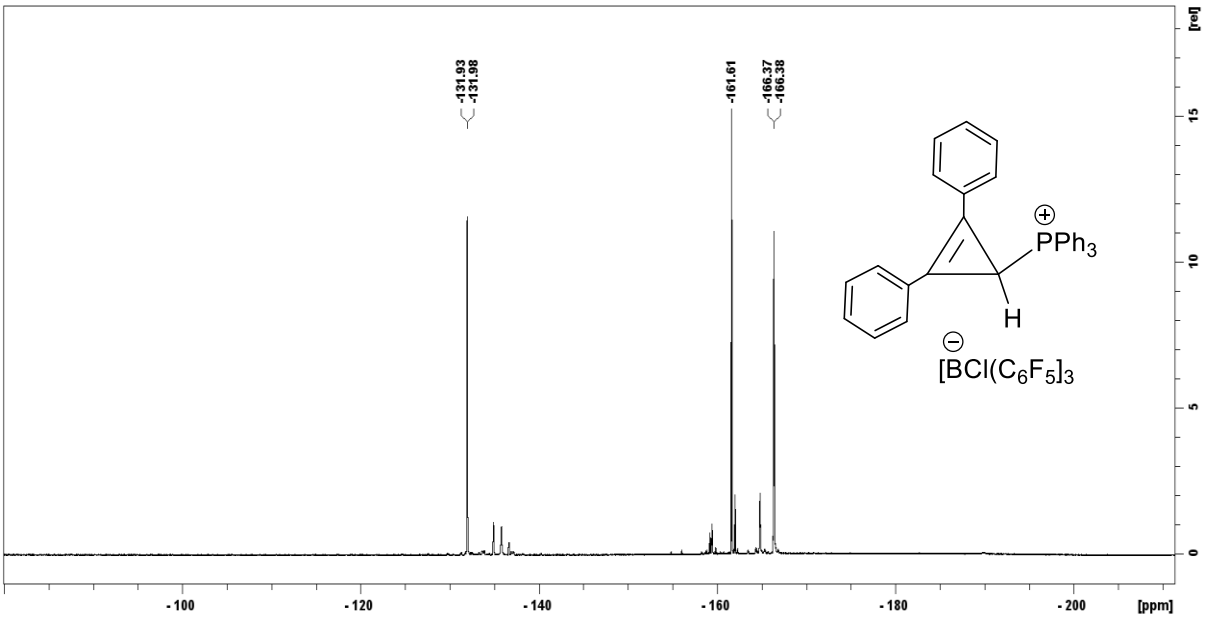


Figure S53. ^{19}F NMR (377 MHz) spectrum of the compound **8** in $CDCl_3$.

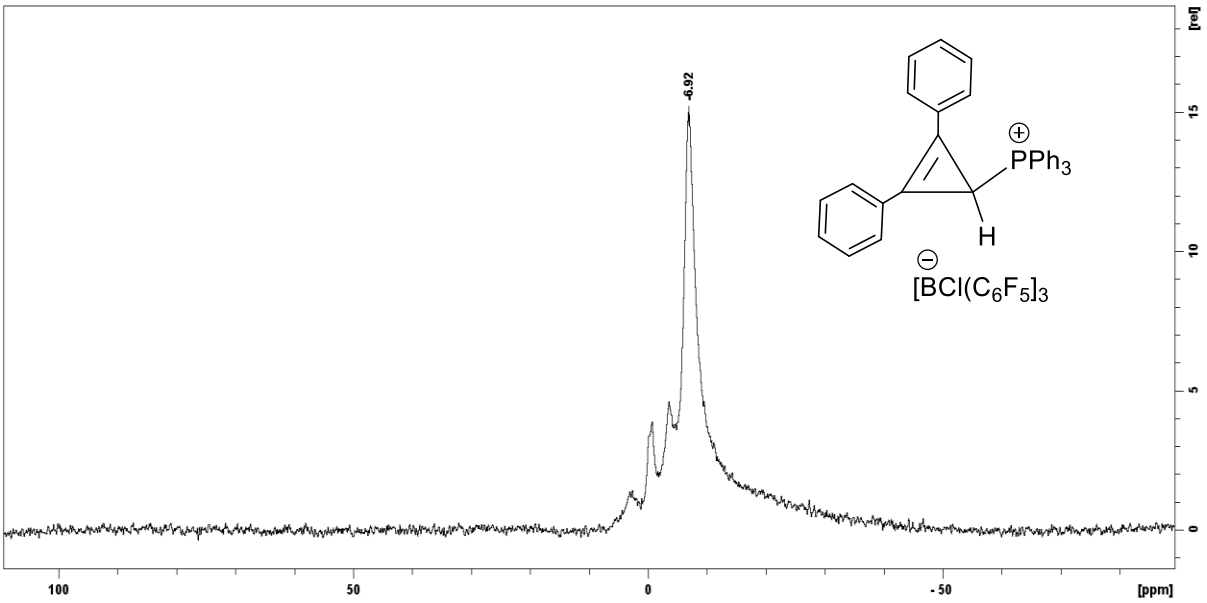


Figure S54. ^{11}B NMR (128 MHz) spectrum of the compound **8** in $CDCl_3$.

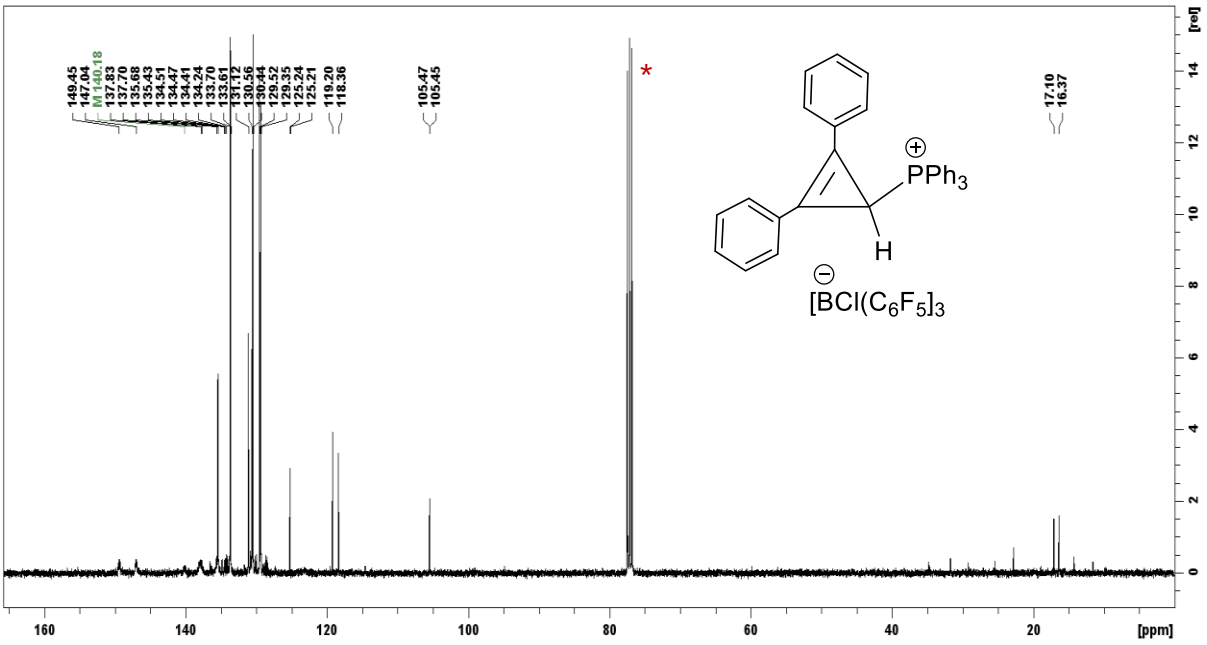


Figure S55. ^{13}C NMR (101 MHz) spectrum of the compound **8** in $CDCl_3$ (*= $CDCl_3$).

Compound 9 and 9′

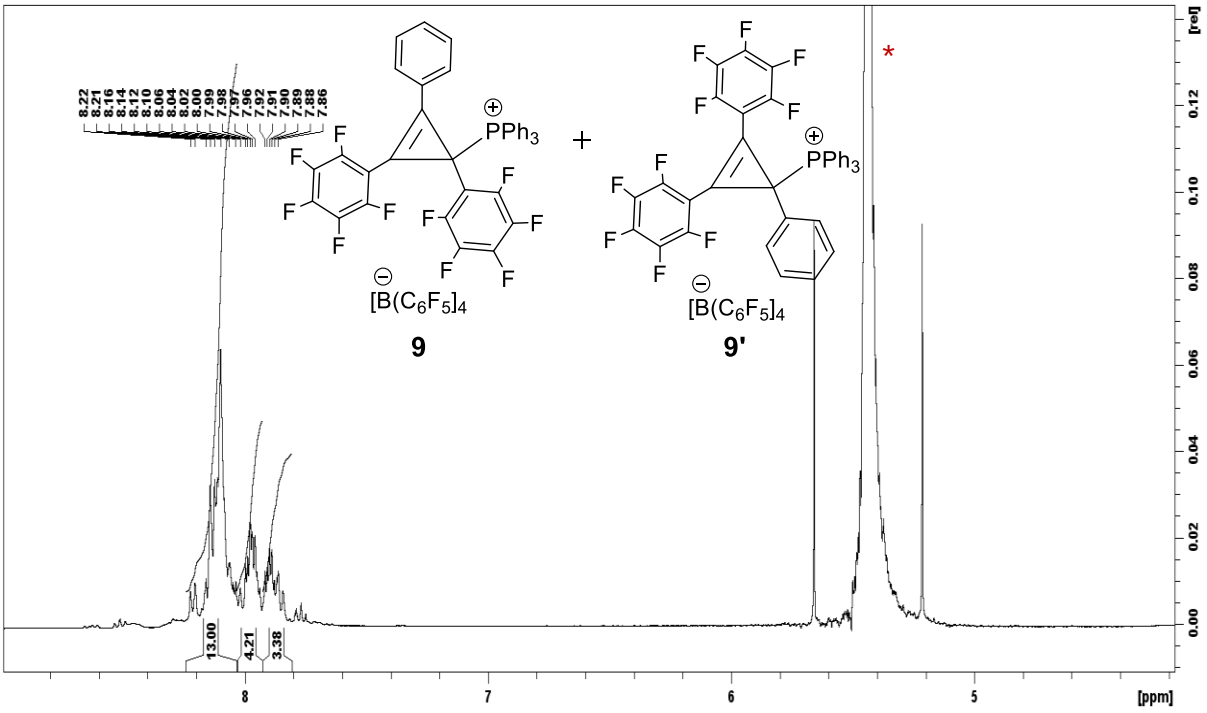


Figure S56. ^{1}H NMR (400 MHz) spectrum of the compounds **9** and **9'** in CD_3CN/DCM (1:2) (*= DCM).

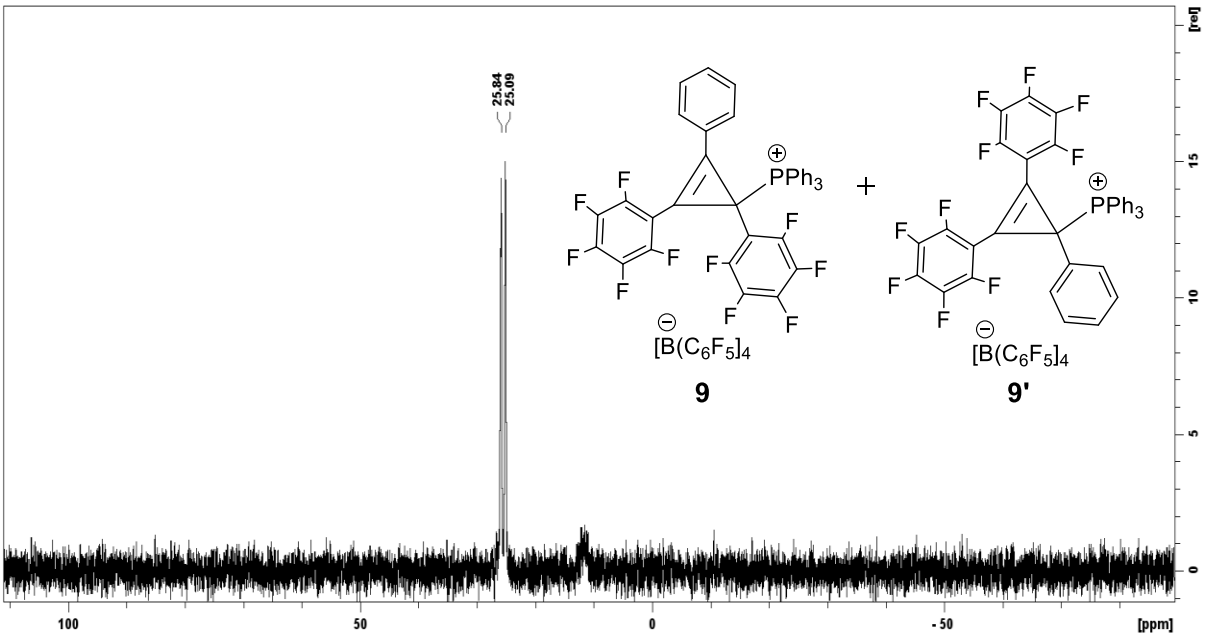


Figure S57. ^{31}P NMR (162 MHz) spectrum of the compounds **9** and **9'** in CD_3CN/DCM (1:2).

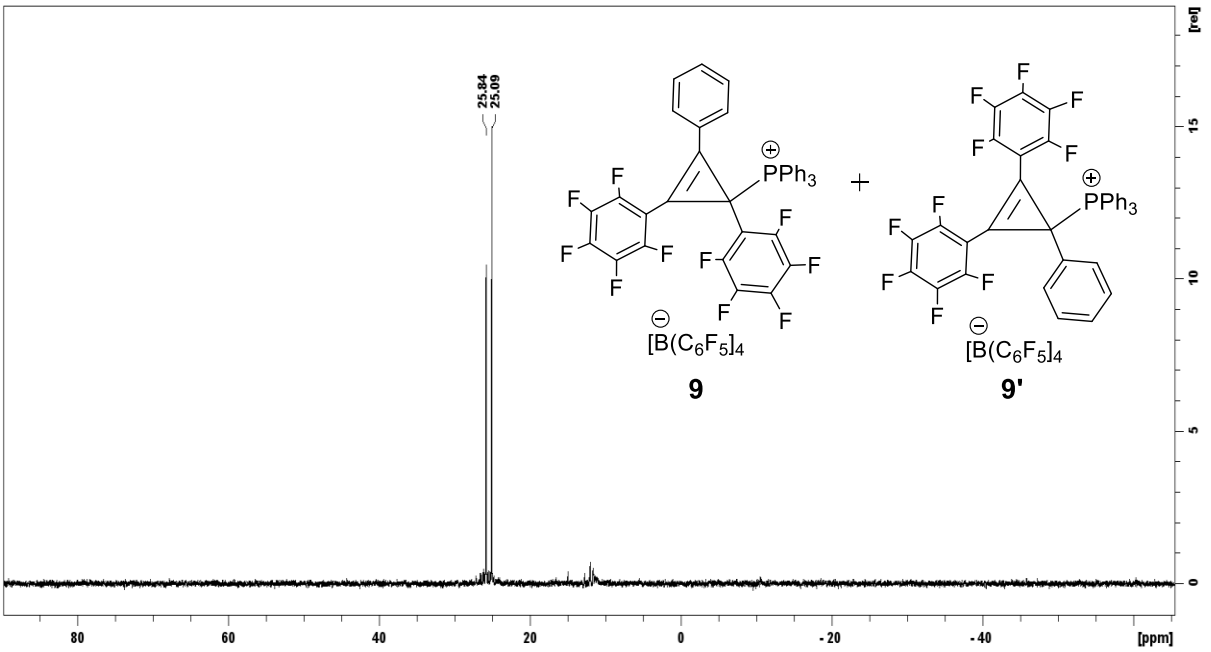


Figure S58. $^{31}P\{^{1}H\}$ NMR (162 MHz) spectrum of the compounds **9** and **9'** in CD_3CN/DCM (1:2).

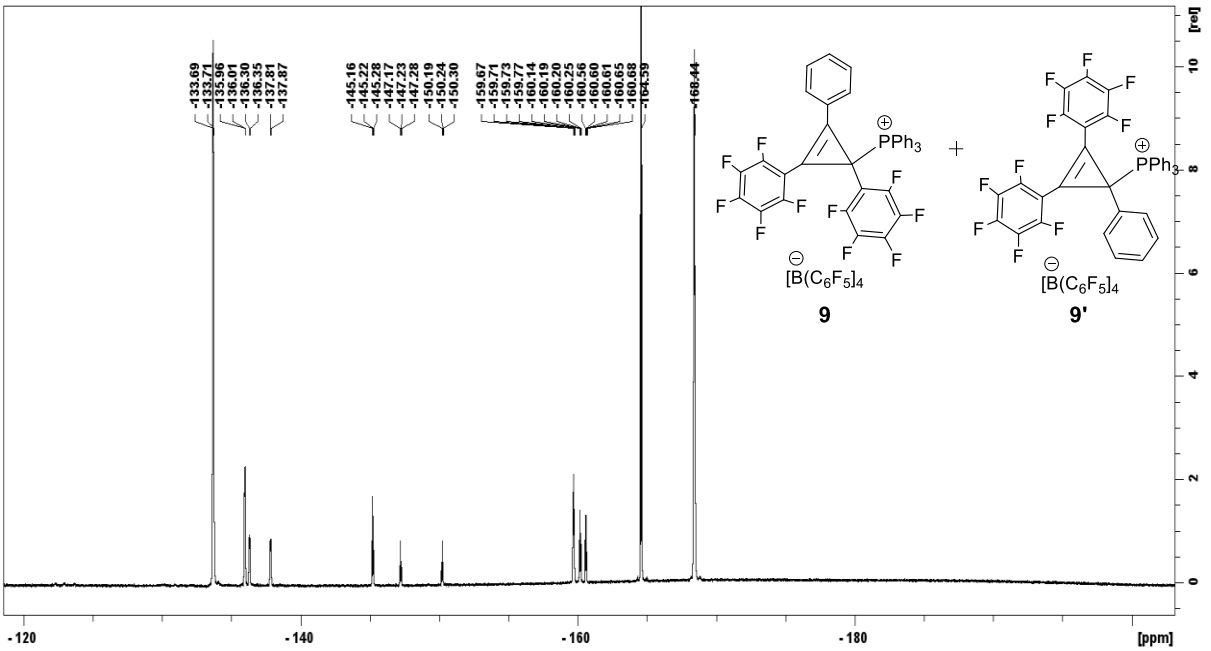


Figure S59. ^{19}F NMR (377 MHz) spectrum of the compounds **9** and **9'** in CD_3CN/DCM (1:2).

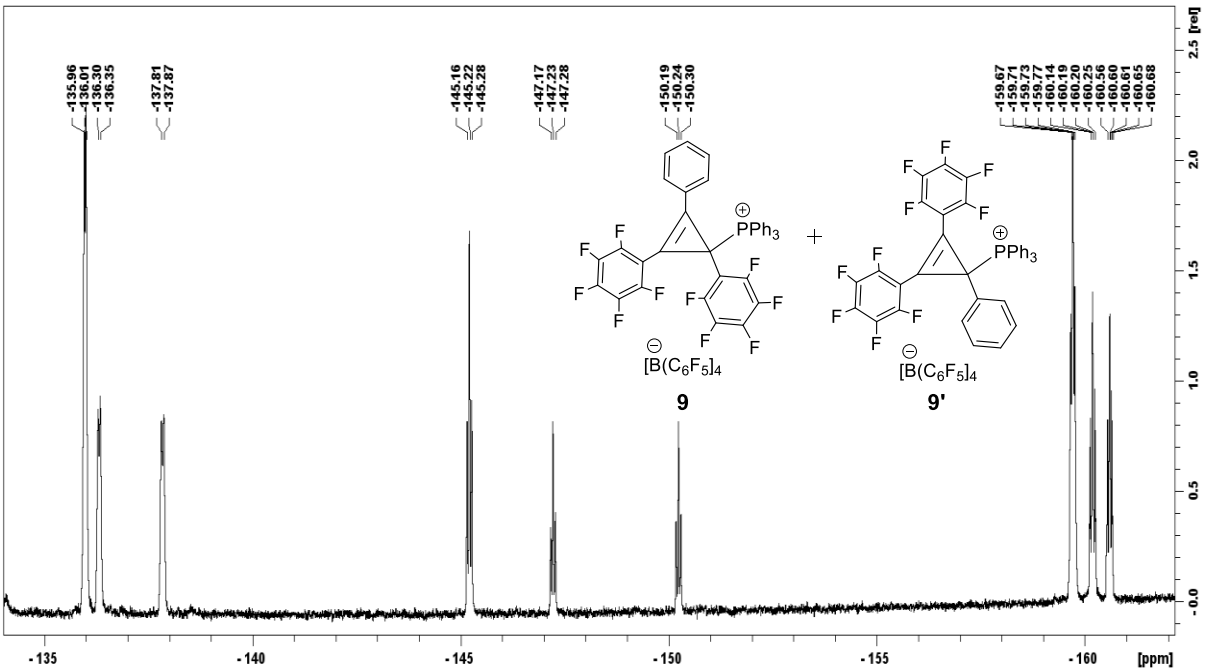


Figure S60. ^{19}F NMR (377 MHz) EXPANSION spectrum (-134 to -162 ppm) of the compounds **9** and **9'**.

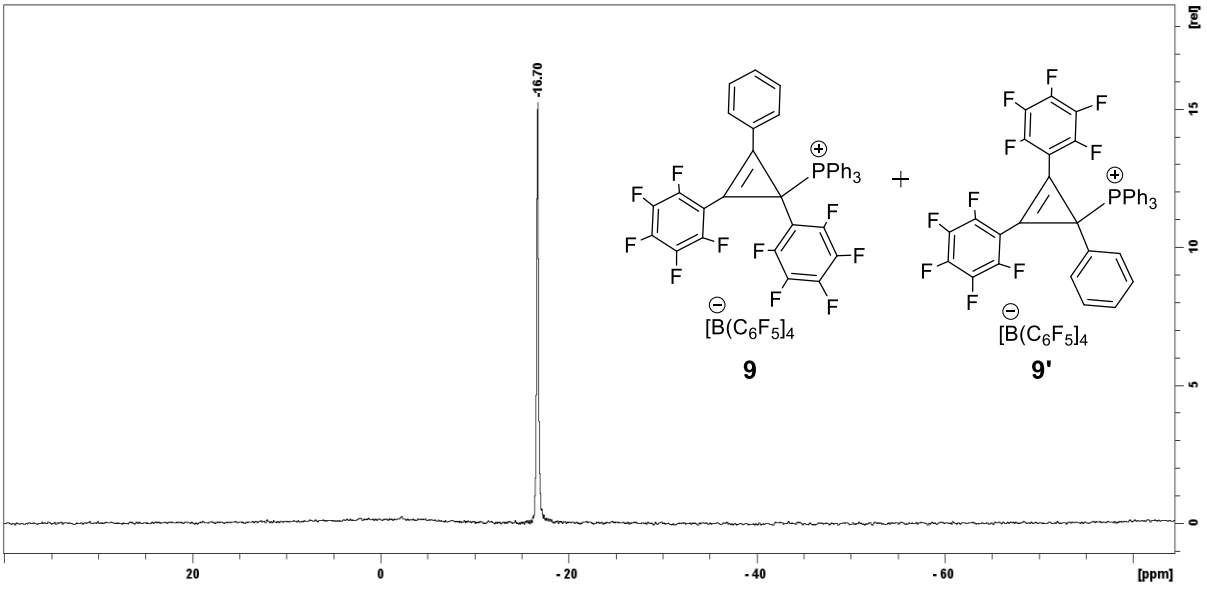


Figure S61. ^{11}B NMR (128 MHz)spectrum of the compounds **9** and **9'** in CD_3CN/DCM (1:2).

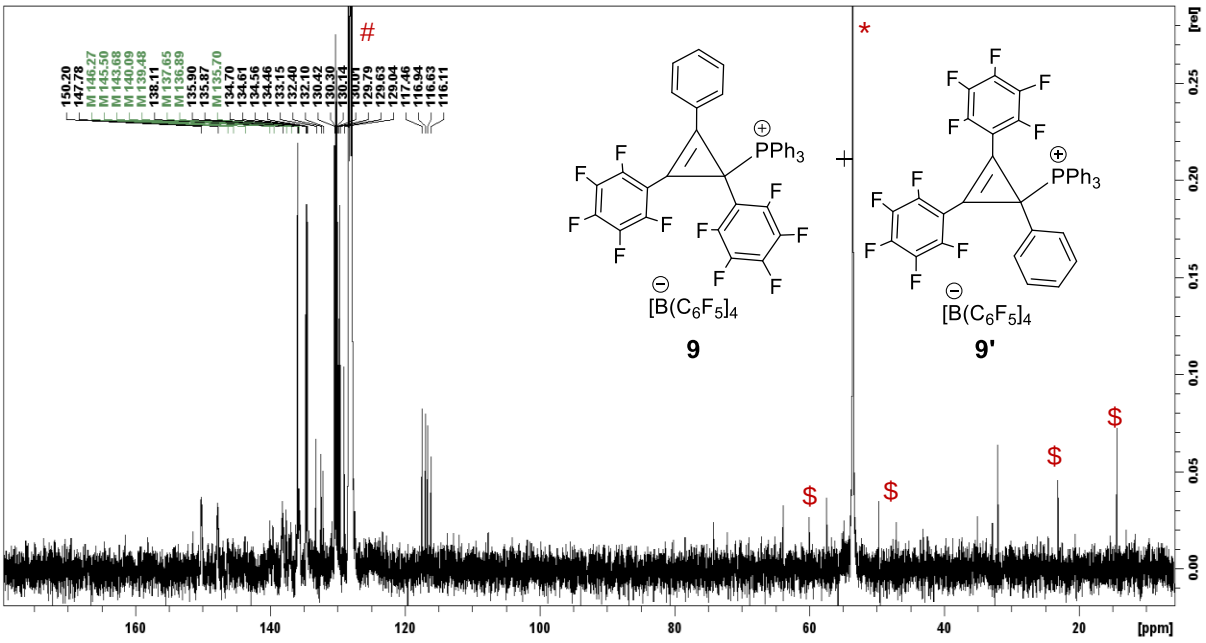


Figure S62. ^{13}C NMR (101 MHz) spectrum of the compounds **9** and **9'** in CD_3CN/DCM (1:2) (*= DCM, #=CD_3CN, $=unidentified impurities).

Compound 10

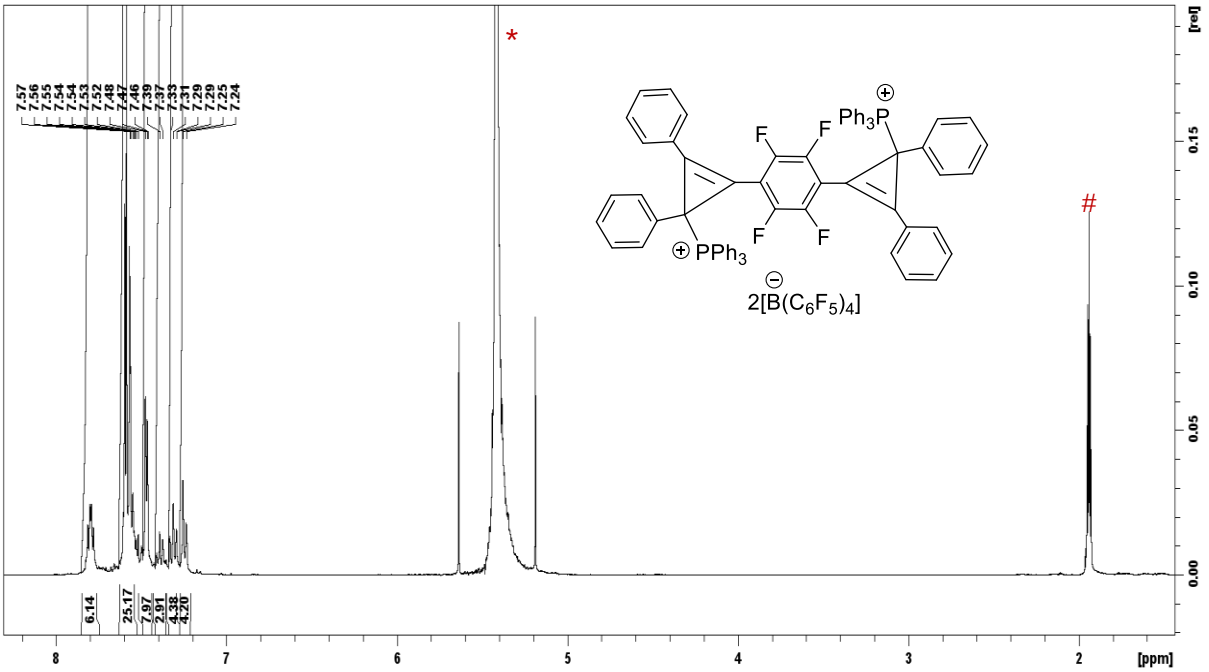


Figure S63. ^{1}H NMR (400 MHz) spectrum of the compound **10** in CD_3CN/DCM (1:2) (*= DCM, #= CD_3CN).

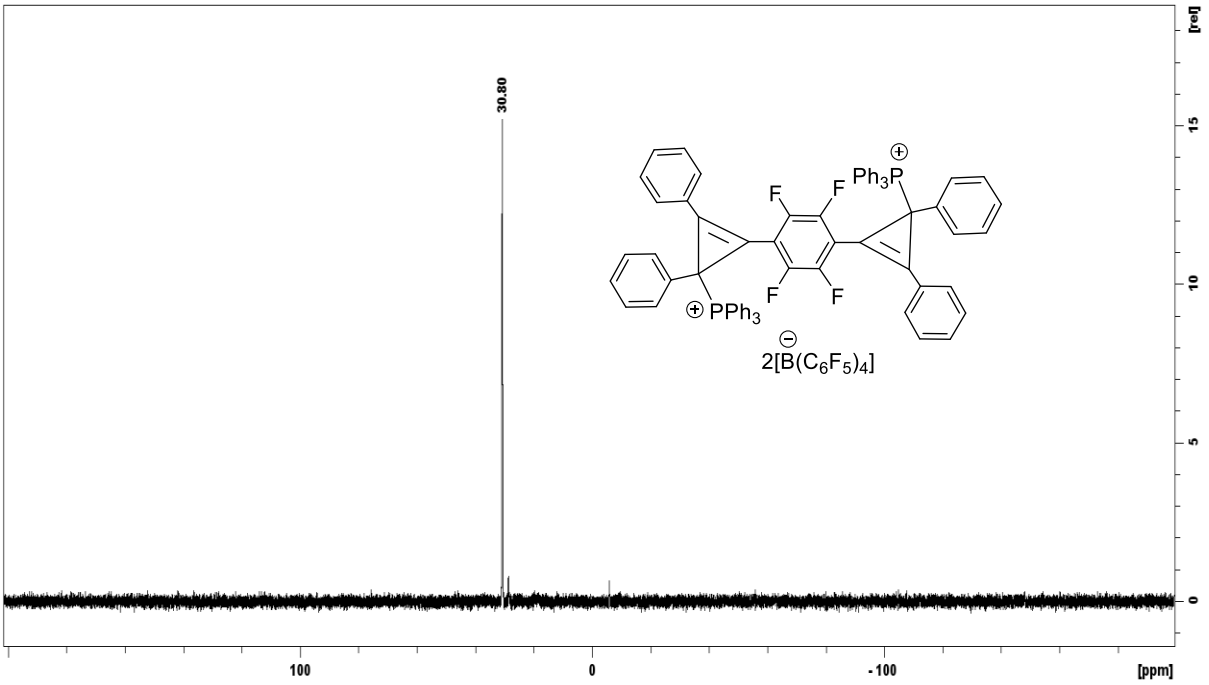


Figure S64. ^{31}P NMR (162 MHz) spectrum of the compound **10** in CD_3CN/DCM (1:2).

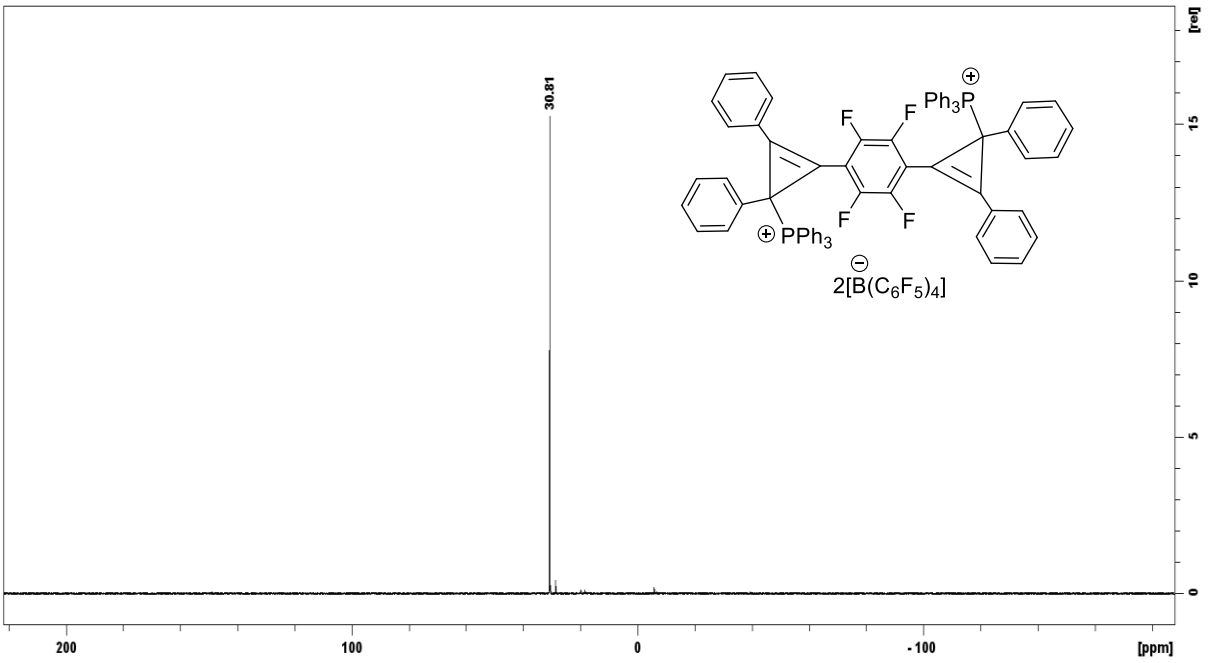


Figure S65. $^{31}P\{^{1}H\}$ NMR (162 MHz) spectrum of the compound **10** in CD_3CN/DCM (1:2).

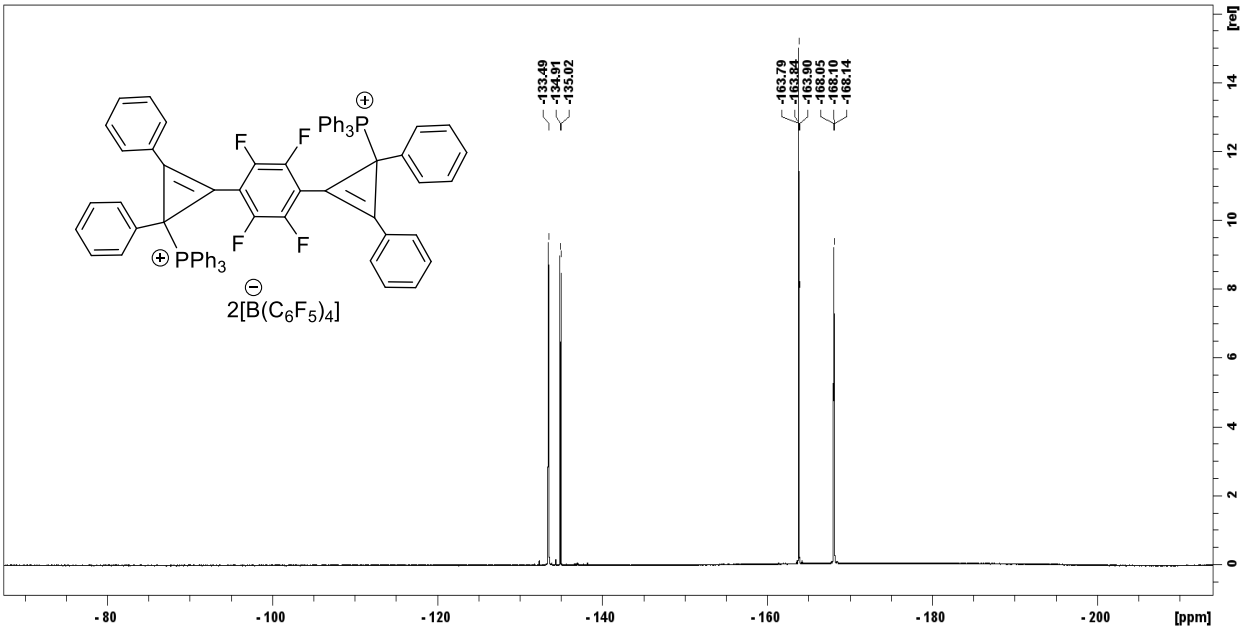


Figure S66. ^{19}F NMR (377 MHz) spectrum of the compound **10** in CD_3CN/DCM (1:2).

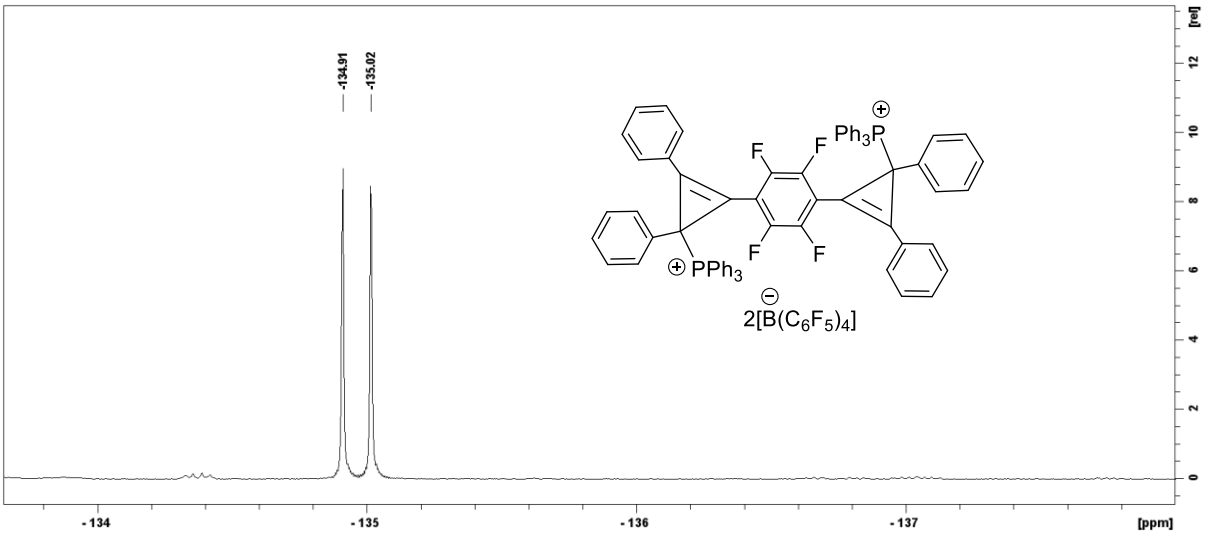


Figure S67. ^{19}F NMR (377 MHz) EXPANSION spectrum (-133 to -137 ppm) of the compound **10**.

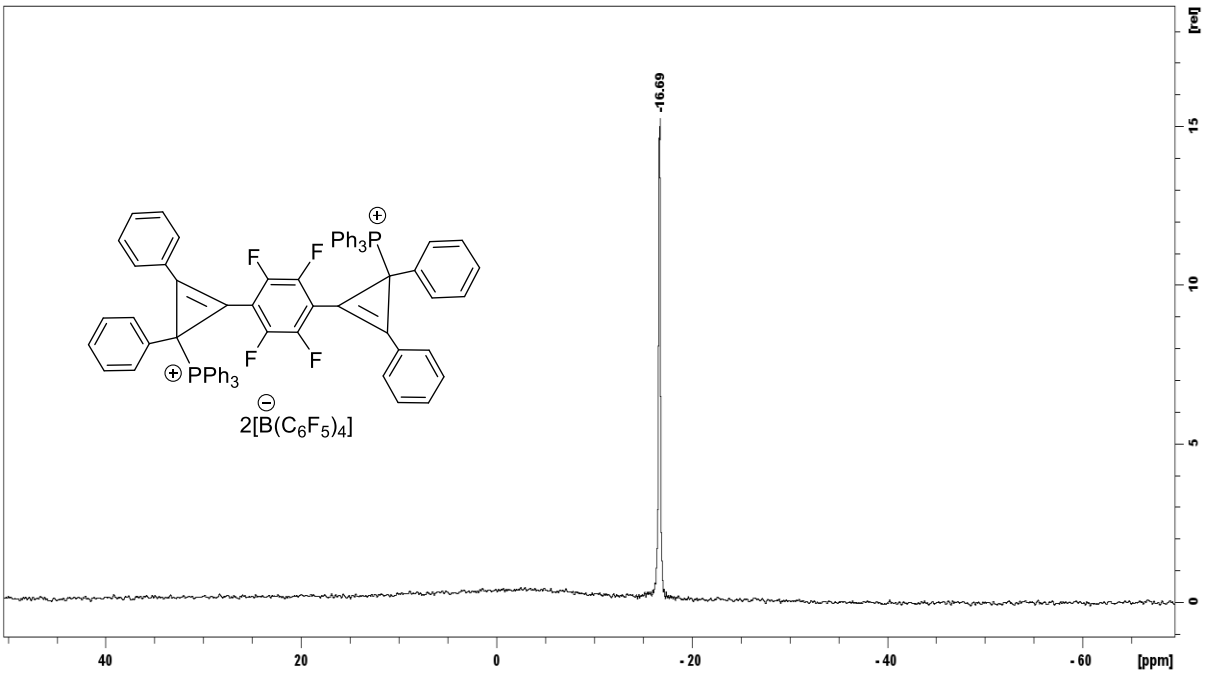


Figure S68. ^{11}B NMR (128 MHz)spectrum of the compound **10** in CD_3CN/DCM (1:2).

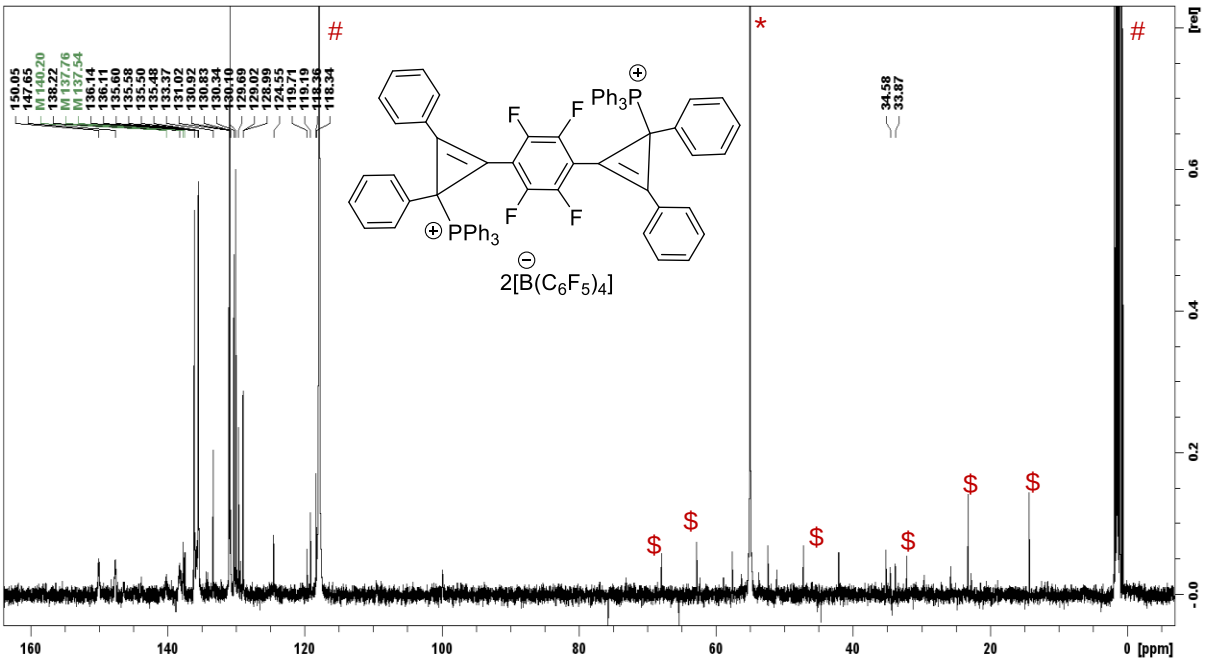


Figure S69. ^{13}C NMR (101 MHz) spectrum of the compound **10** in CD_3CN/DCM (1:2) (*= DCM, #=CD_3CN, $=unidentified impurities).

Compound 11

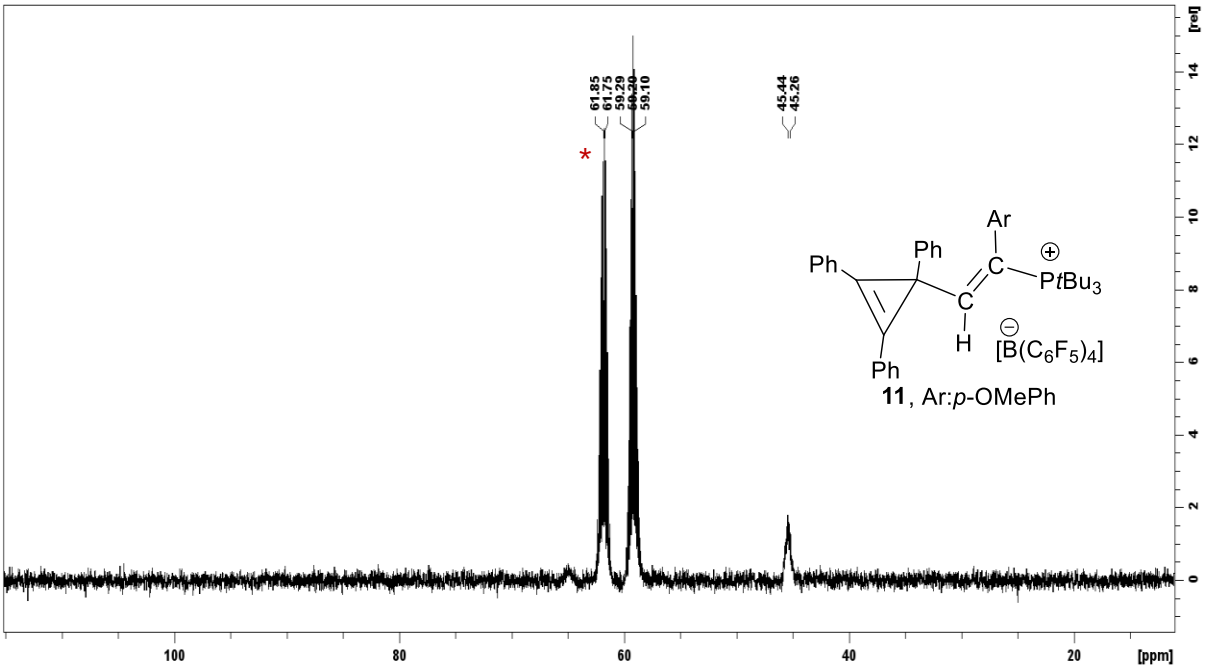


Figure S70. ^{31}P NMR (162 MHz) spectrum of the compound **11** in DCM (*= $[tBu_3PH][B(C_6F_5)_4]$).

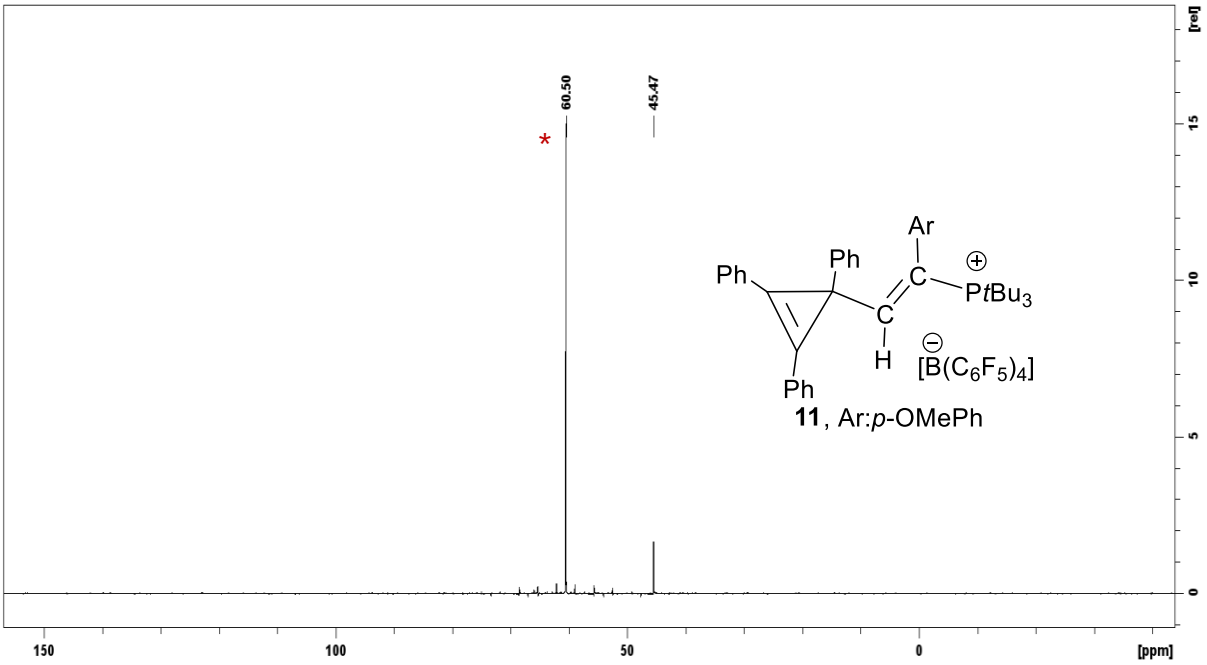


Figure S71. $^{31}P\{^1H\}$ NMR (162 MHz) spectrum of the compound **11** in DCM (*= $[tBu_3PH][B(C_6F_5)_4]$).

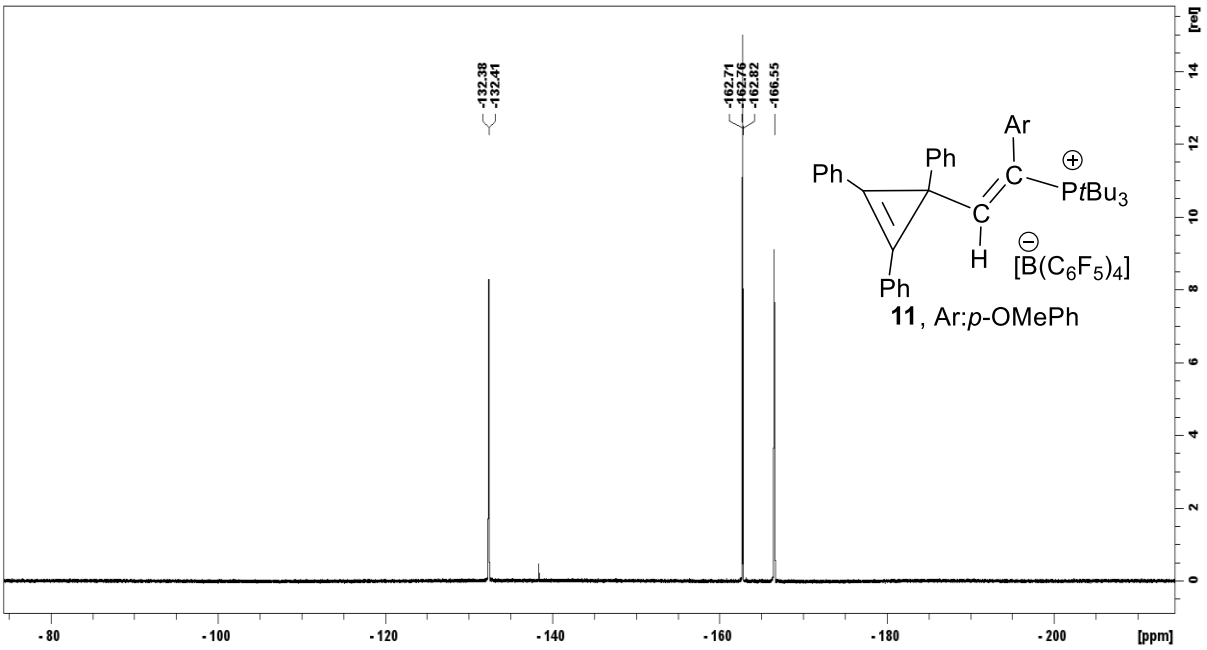


Figure S72. ^{19}F NMR (377 MHz) spectrum of the compound **11** in DCM.

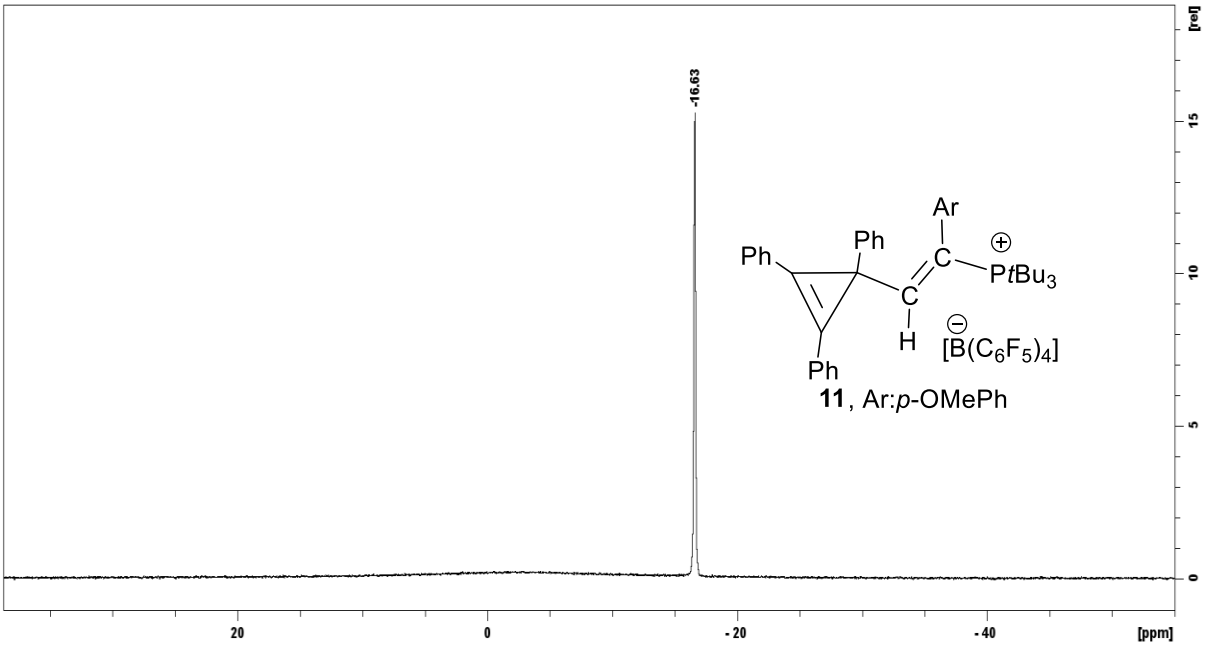


Figure S73. ^{11}B NMR (128 MHz)spectrum of the compound **11** in DCM.

Compound 12

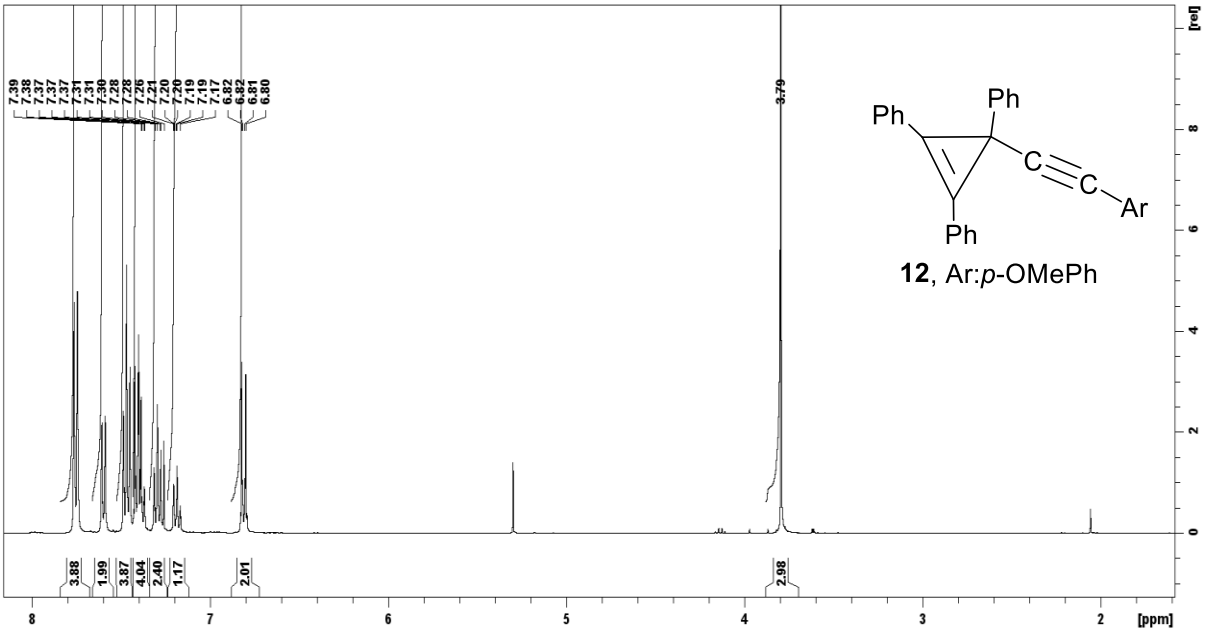


Figure S74. ^{1}H NMR (400 MHz) spectrum of the compound **12** in $CDCl_3$ (*= $CDCl_3$).

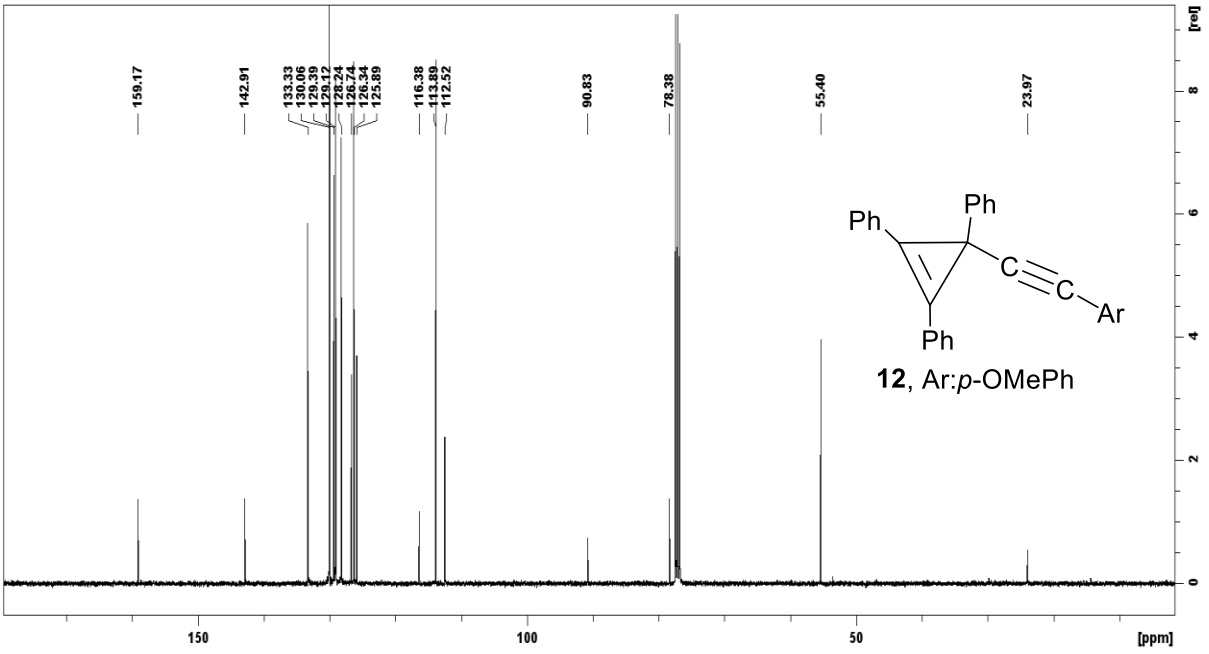


Figure S75. ^{13}C NMR (101 MHz) spectrum of the compound **12** in $CDCl_3$ (*= $CDCl_3$).

Compound 13

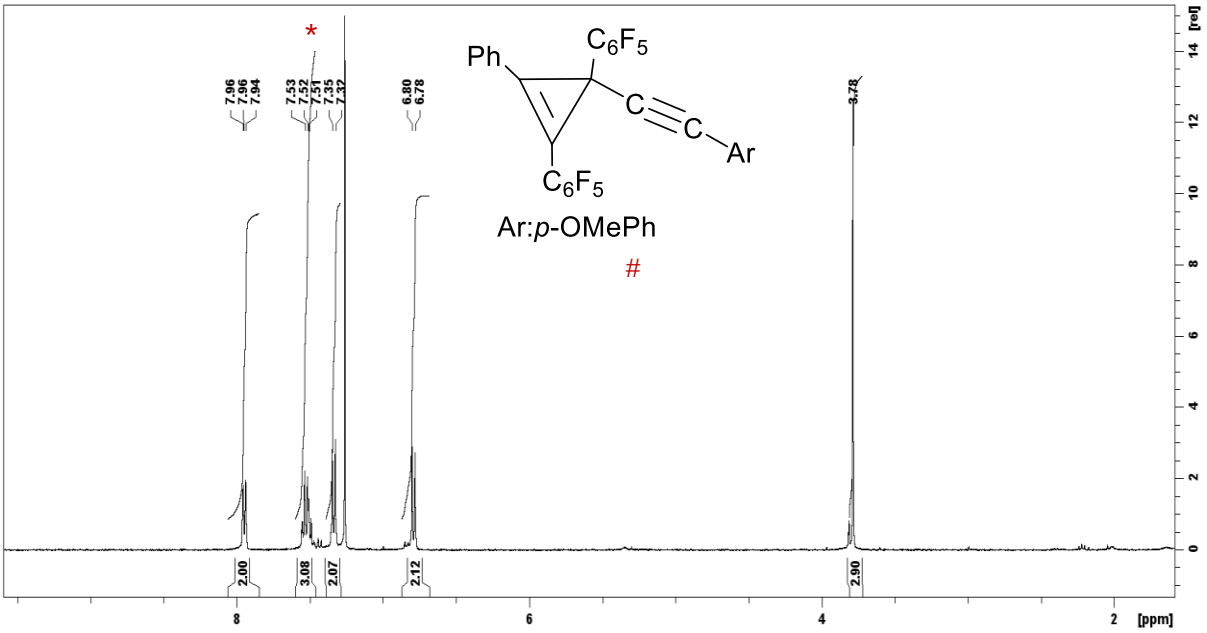


Figure S76. ^{1}H NMR (400 MHz) spectrum of the compound **13** in $CDCl_3$ (*= $CDCl_3$, #=DCM).

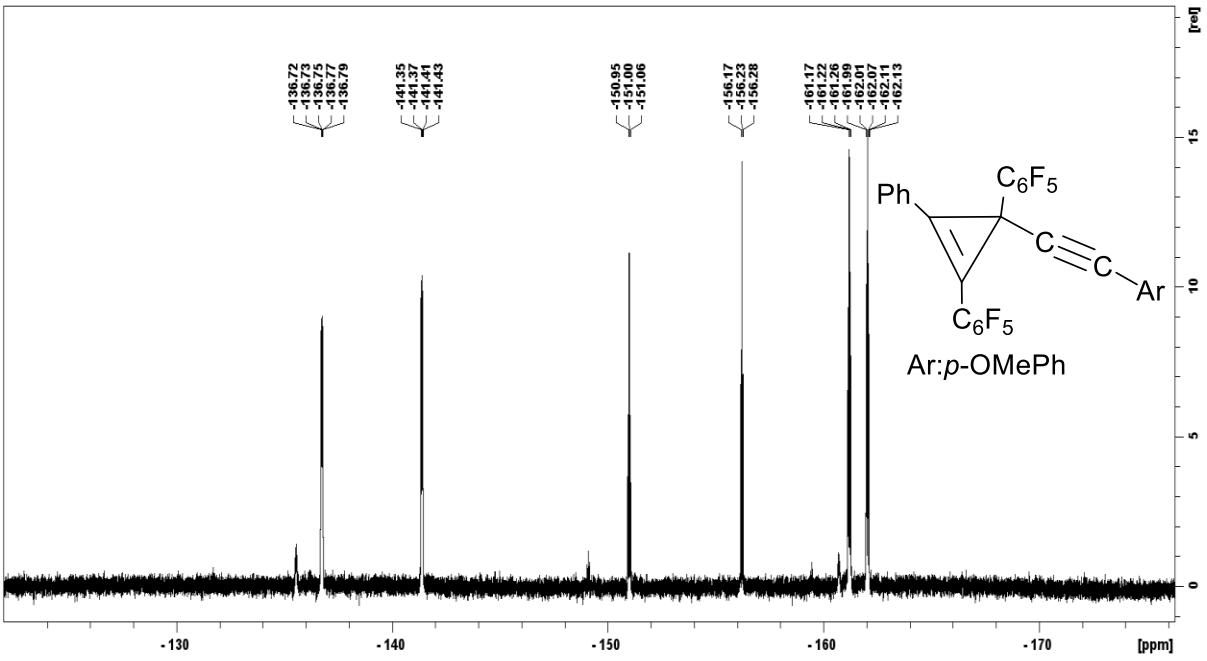


Figure S77. ^{19}F NMR (377 MHz) spectrum of the compound **13** in $CDCl_3$ (*= $CDCl_3$).

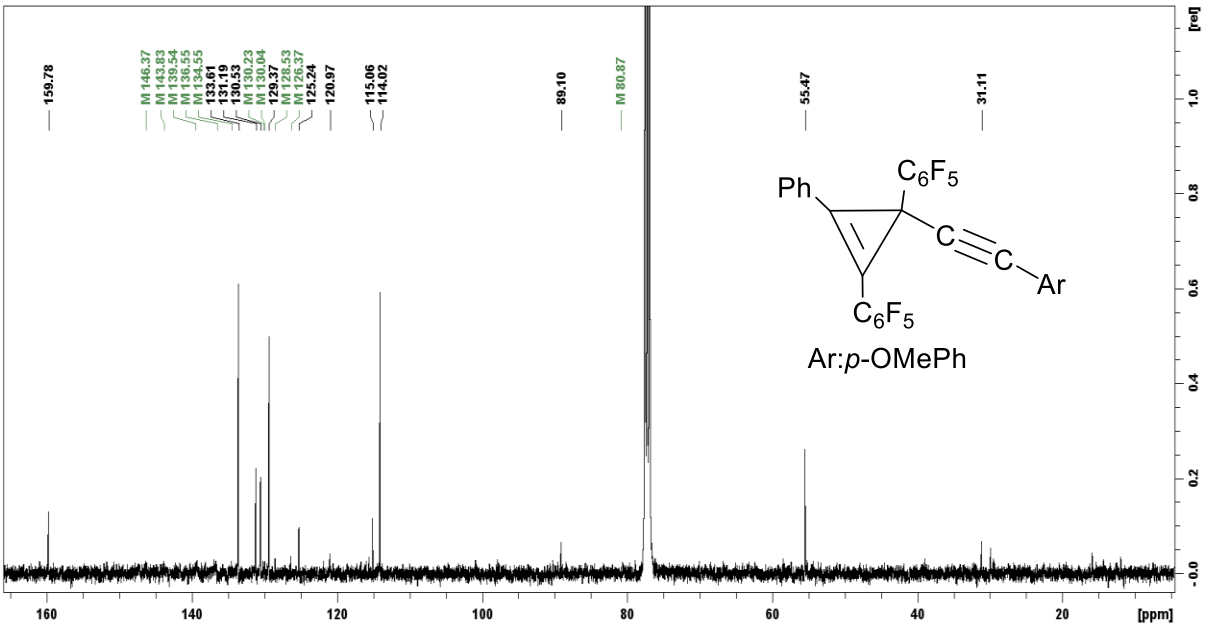


Figure S78. ^{13}C NMR (101 MHz) spectrum of the compound **13** in $CDCl_3$ (*= $CDCl_3$).

Compound 14

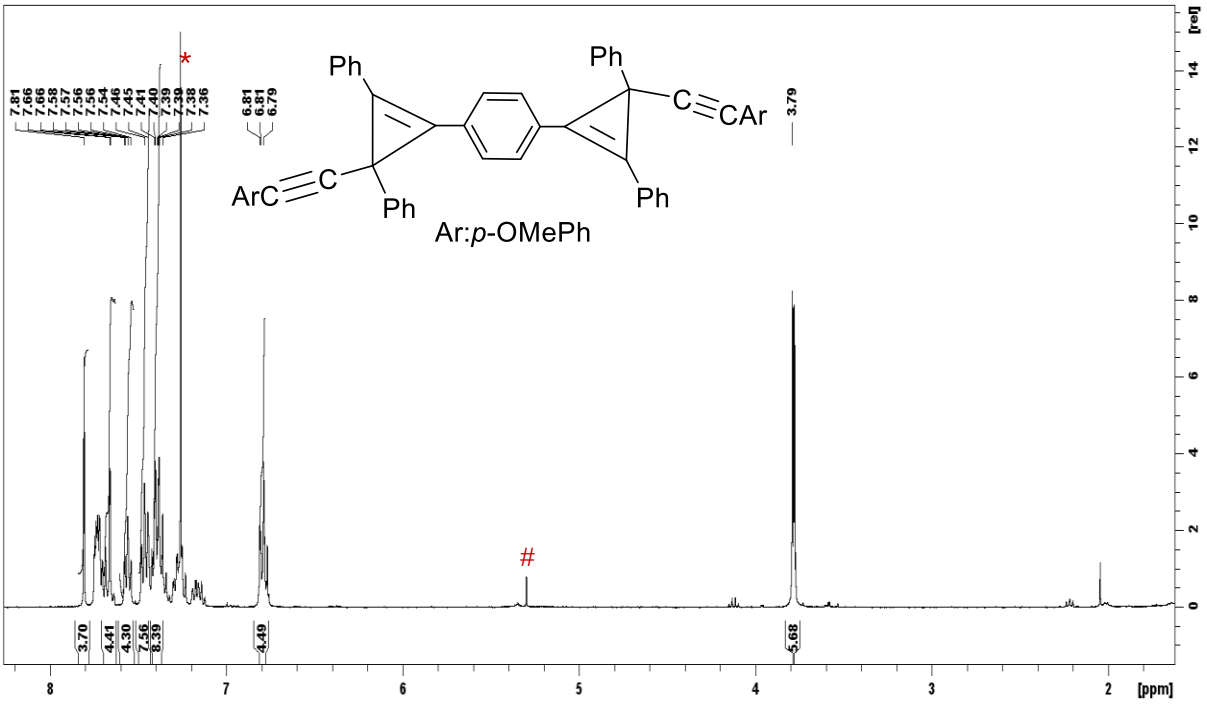
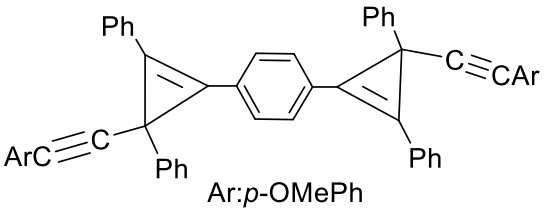


Figure S79. ^{1}H NMR (400 MHz) spectrum of the compound **14** in $CDCl_3$ (*= $CDCl_3$, #=DCM).



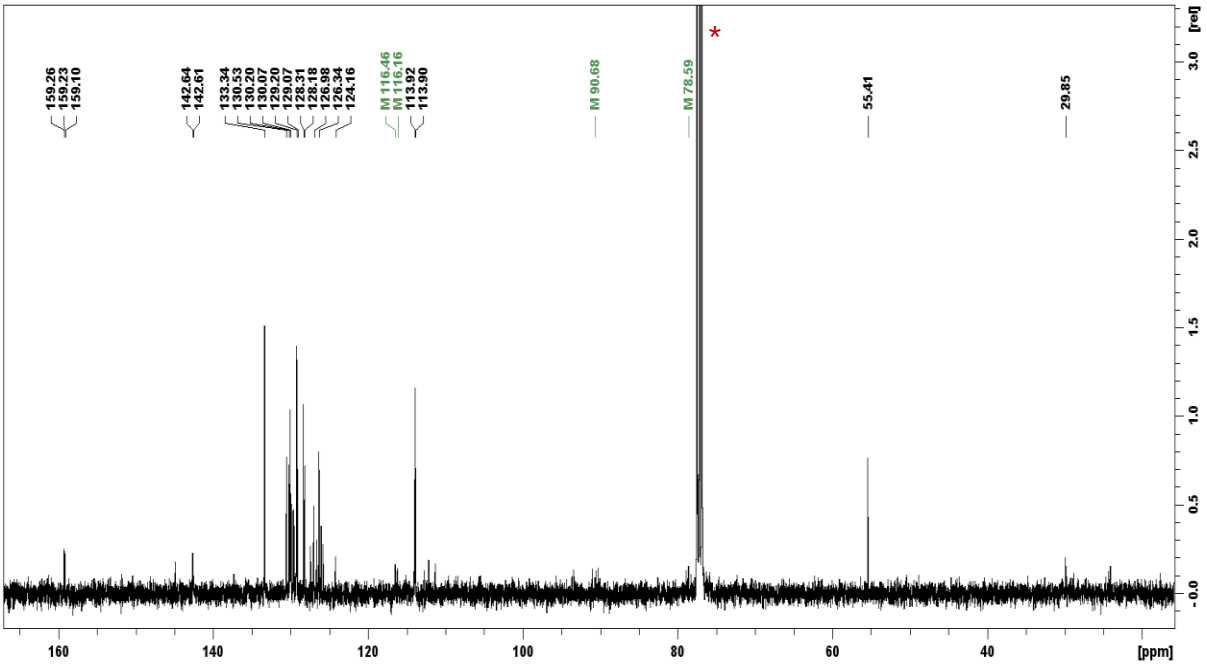


Figure S80. ^{13}C NMR (101 MHz) spectrum of the compound **14** in $CDCl_3$ (*= $CDCl_3$).

Compound 15

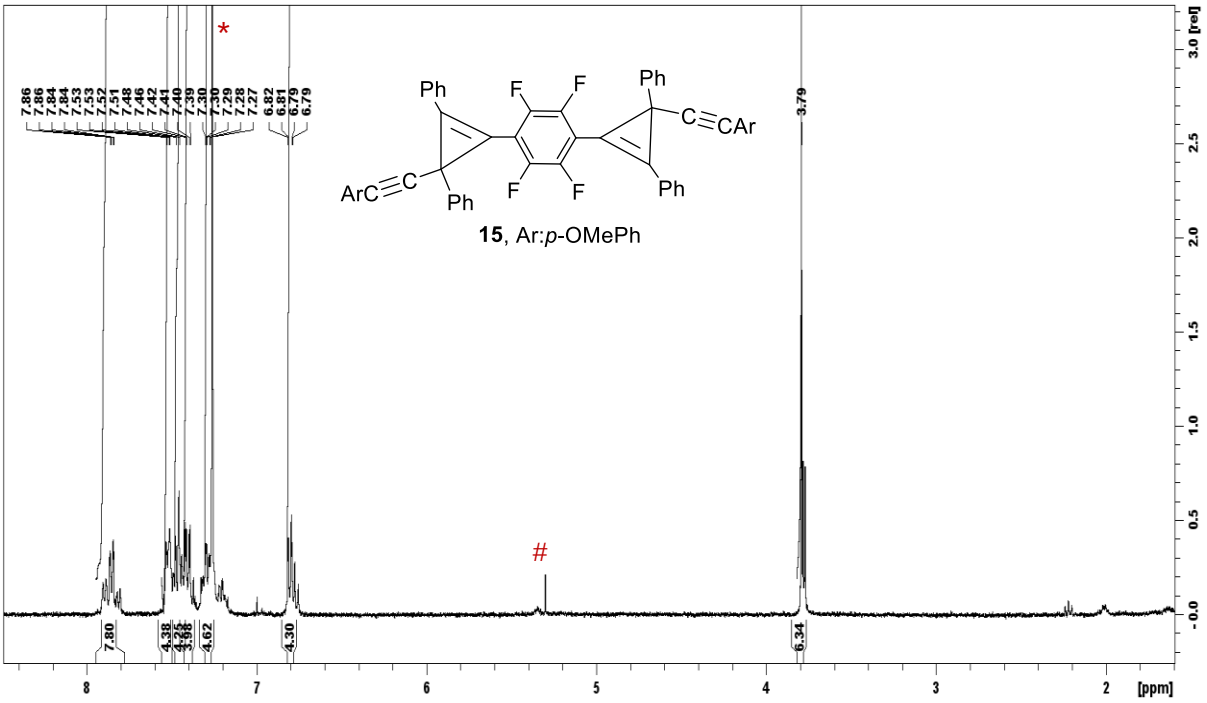


Figure S81. ^{1}H NMR (400 MHz) spectrum of the compound **15** in $CDCl_3$ (*= $CDCl_3$, #=DCM).

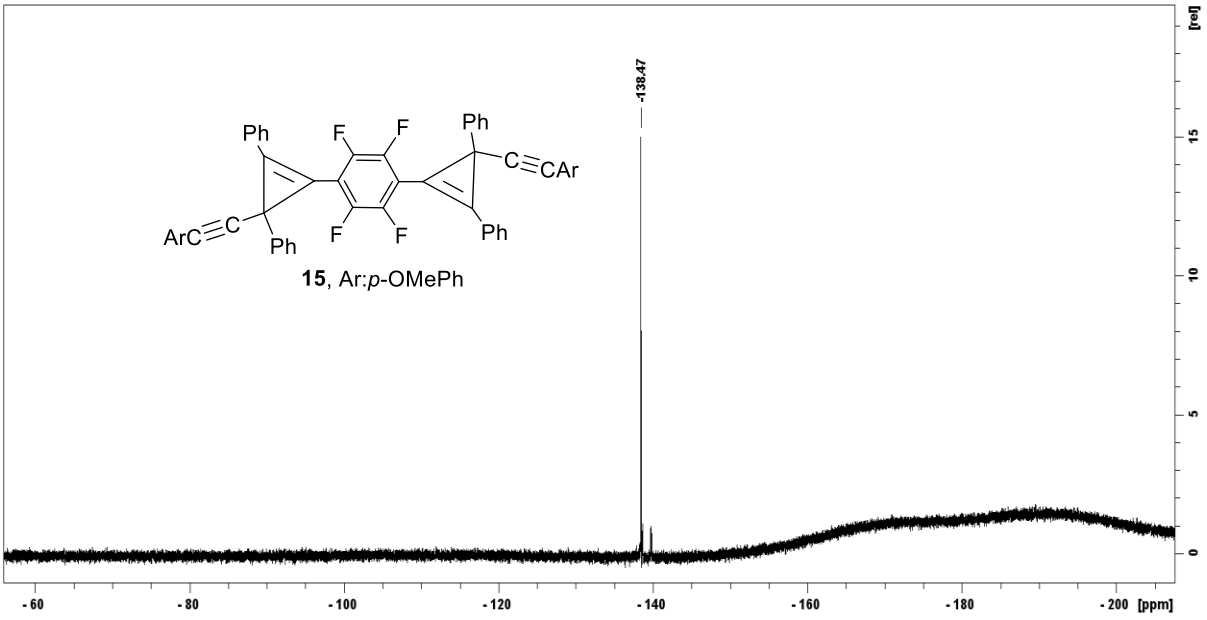


Figure S82. ^{19}F NMR (377 MHz) spectrum of the compound **15** in $CDCl_3$ (*= $CDCl_3$).

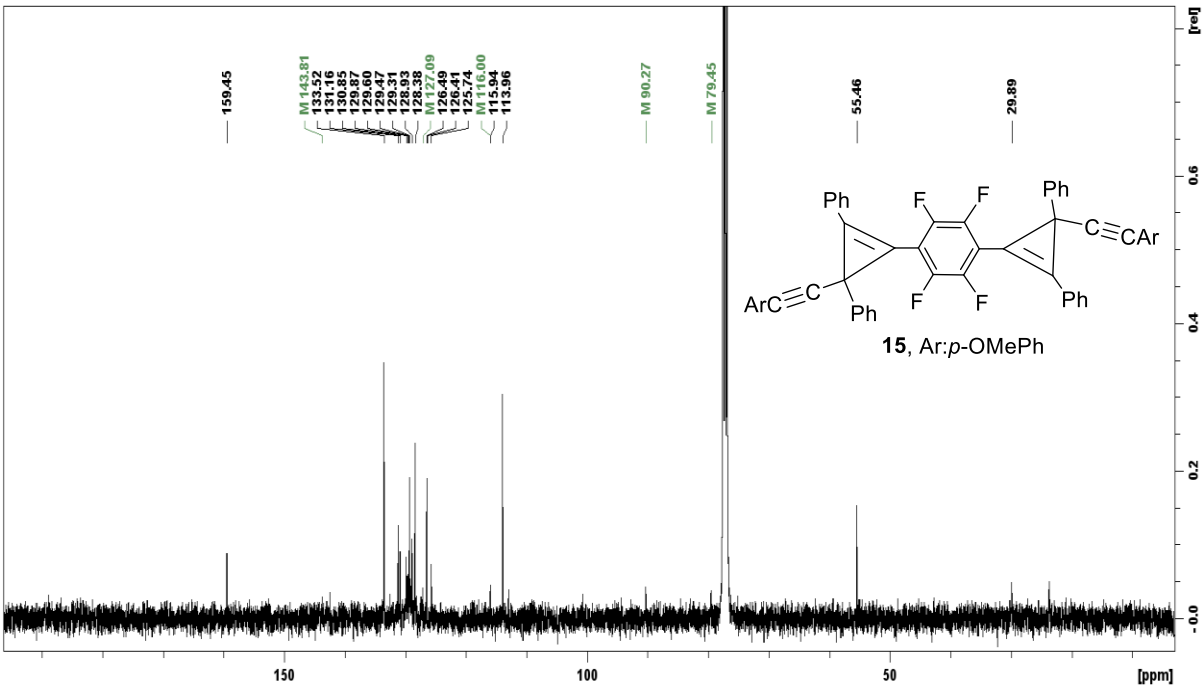


Figure S83. ^{13}C NMR (101 MHz) spectrum of the compound **15** in $CDCl_3$ (*= $CDCl_3$).

Compound 16

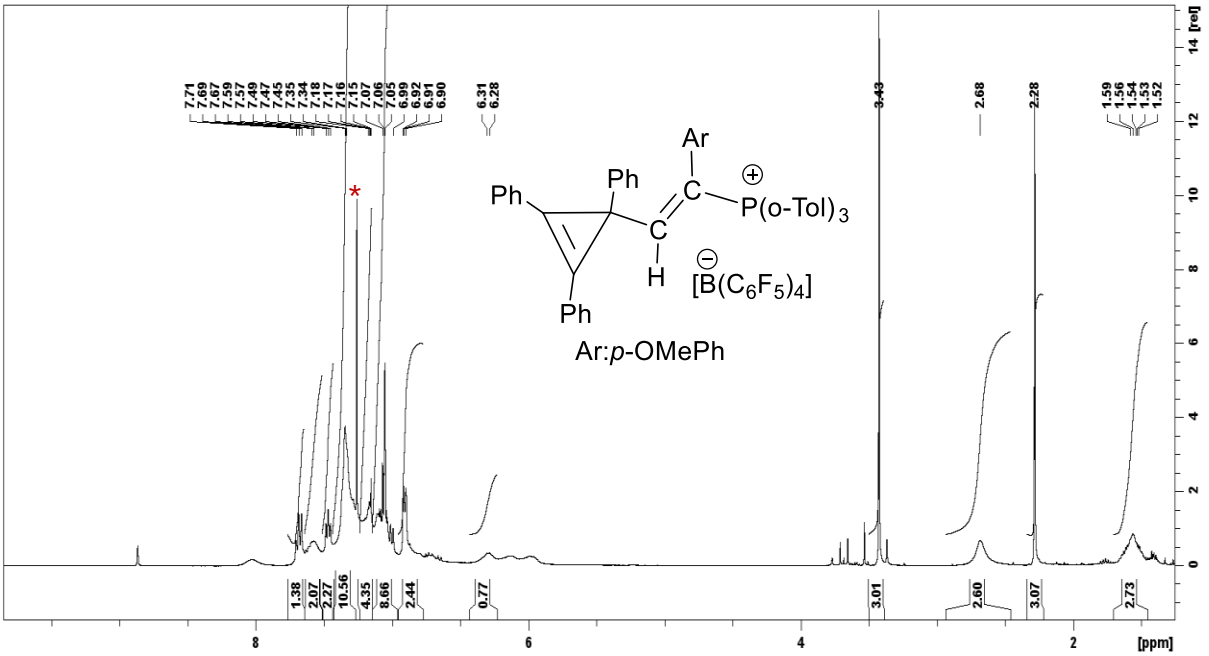


Figure S84. ^{1}H NMR (400 MHz) spectrum of the compound **16** in $CDCl_3$ (*= $CDCl_3$).

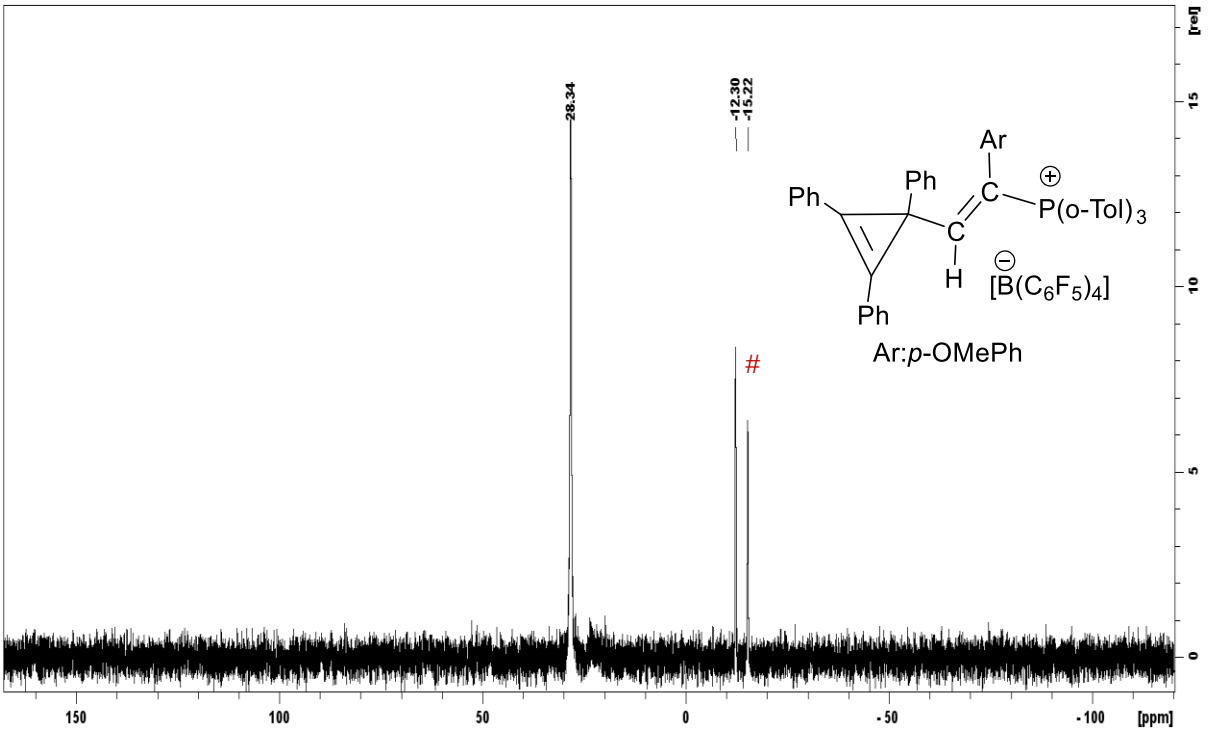


Figure S85. ^{31}P NMR (126 MHz) spectrum of the compound **16** in $CDCl_3$ (#=[HP(*o*-Tol)$_3$][B(C$_6$F$_5$)$_4$]).

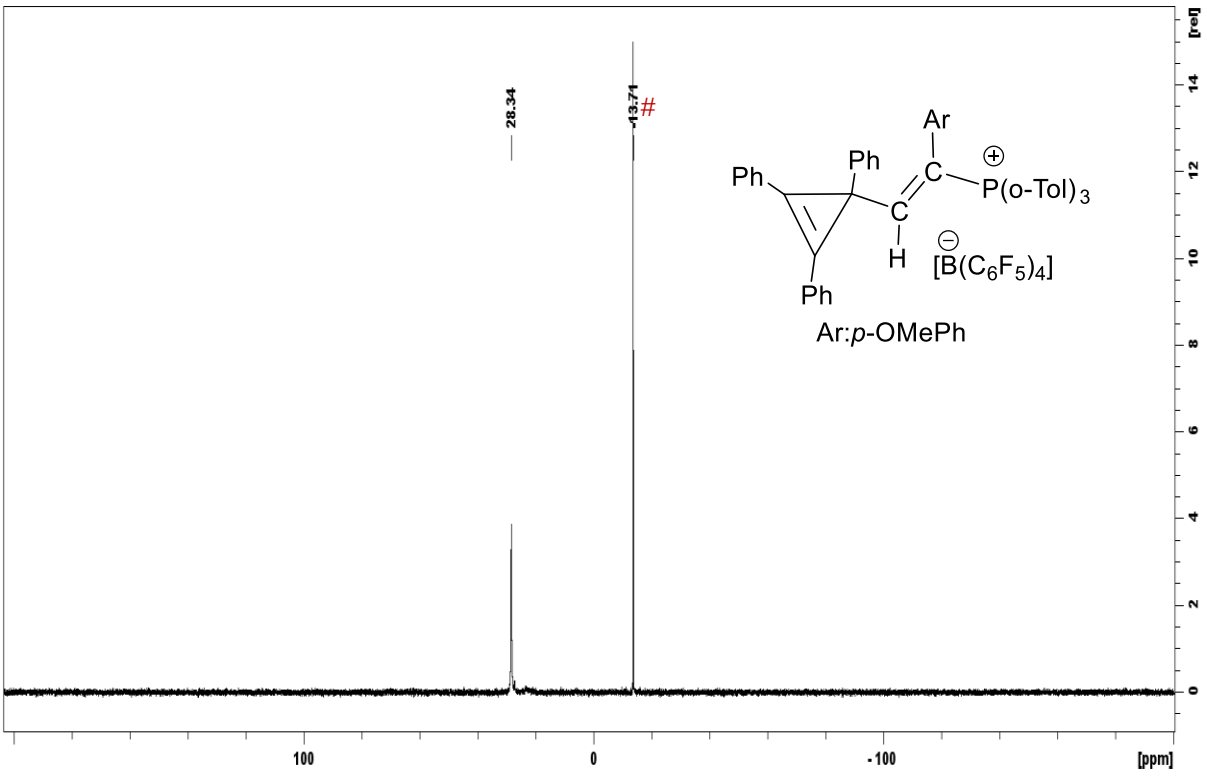


Figure S86. $^{31}P\{^{1}H\}$ NMR (126 MHz) spectrum of the compound **16** in $CDCl_3$ (#=[HP(*o*-Tol)$_3$][B(C_6F_5)$_4$]).

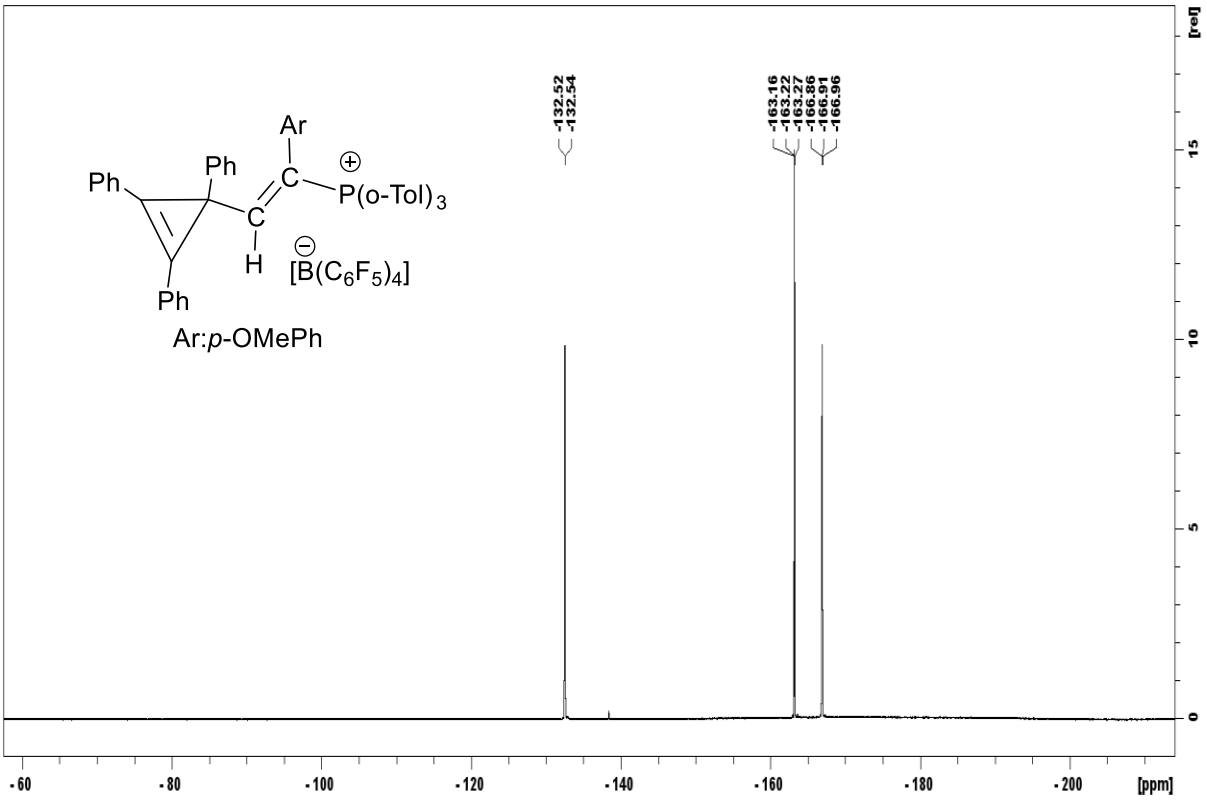


Figure S87. ^{19}F NMR (377 MHz) spectrum of the compound **16** in $CDCl_3$.

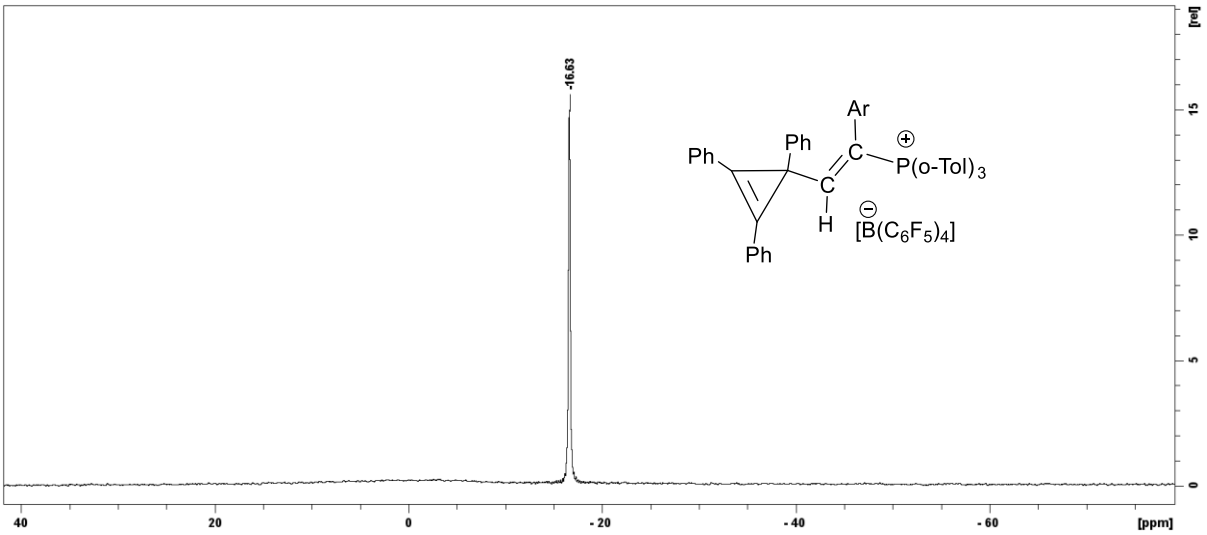


Figure S88. ^{11}B NMR (127 MHz) spectrum of the compound **16** in $CDCl_3$.

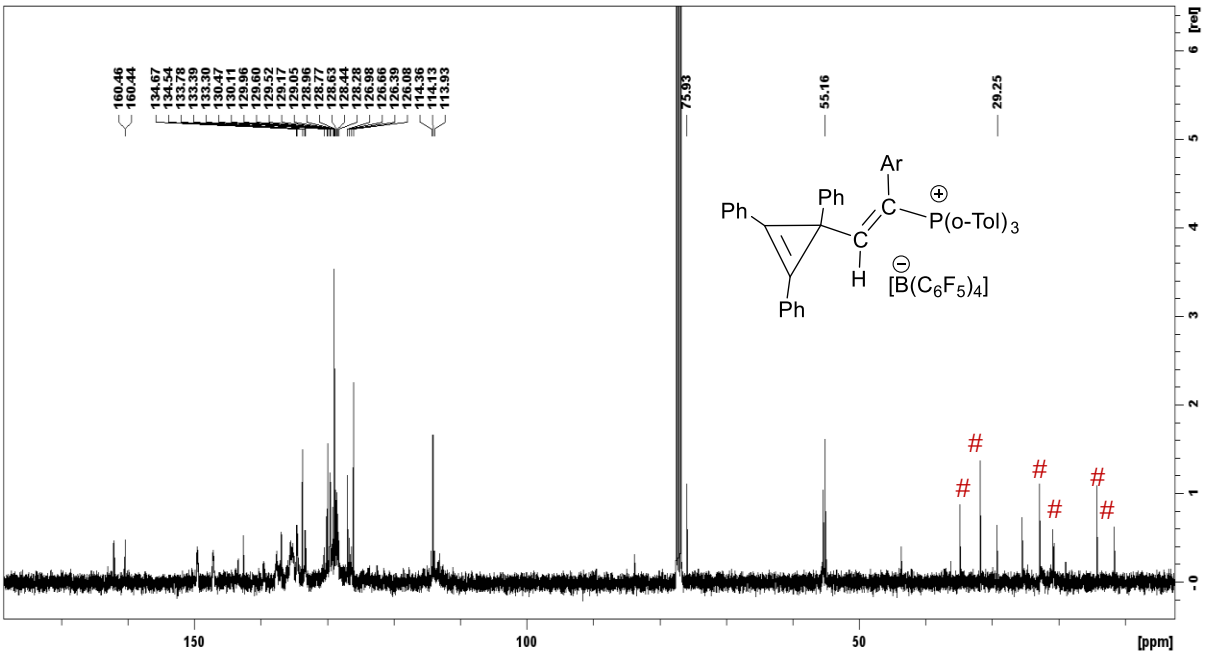


Figure S89. ^{13}C NMR (101 MHz) spectrum of the compound **16** in $CDCl_3$ (*= $CDCl_3$;#= unidentified impurities and $[HP(o\text{-Tol})_3][B(C_6F_5)_4]$).

HRMS spectra of all the compounds

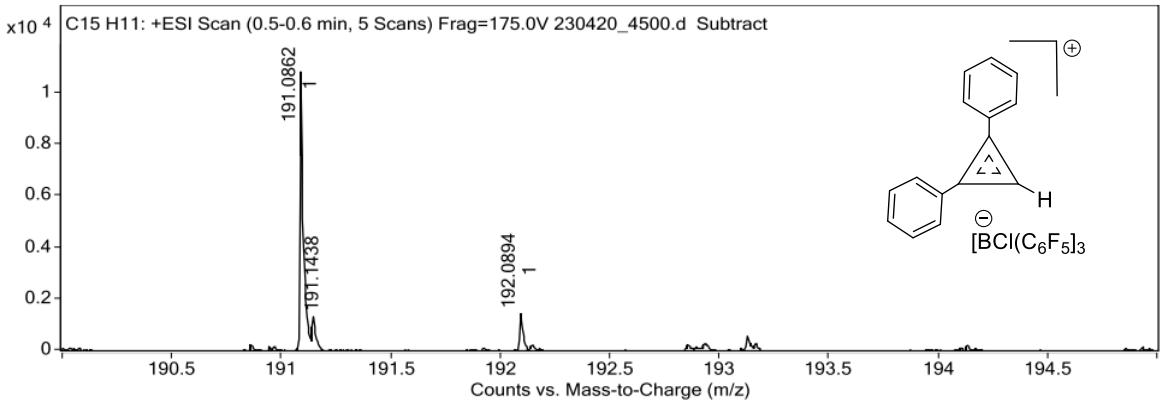
Compound 1

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	191.0862	C15 H11

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
191.0862	C15 H11	191.0855	0.7	3.7	10.5	96.88
191.1438	C13 H19 O	191.1430	0.8	4.2	4.5	75.33



Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	191.0862	191.0855	0.7	100.0	100.0	0.0
2	192.0894	192.0889	0.5	14.5	16.4	1.9
3	193.0941	193.0923	1.8	1.2	1.2	0.0

Figure S90. HRMS (ESI) spectrum of the compound **1**.

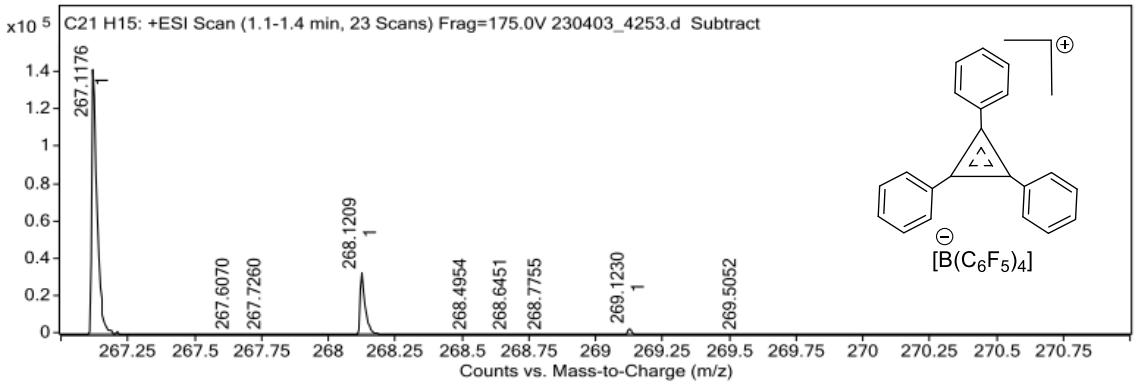
Compound 2b

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	267.1176	C21 H15

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
267.1176	C21 H15	267.1168	0.8	3.0	14.5	97.61
267.1176	C9 H19 N2 O7	267.1187	-1.1	-4.1	1.5	76.93
267.1176	C10 H15 N6 O3	267.1200	-2.4	-9.0	6.5	69.11



Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	267.1176	267.1168	0.8	100.0	100.0	0.0
2	268.1209	268.1202	0.7	21.7	22.9	1.2
3	269.1230	269.1236	-0.6	2.3	2.5	0.2

Figure S91. HRMS (ESI) spectrum of the compound **2b**.

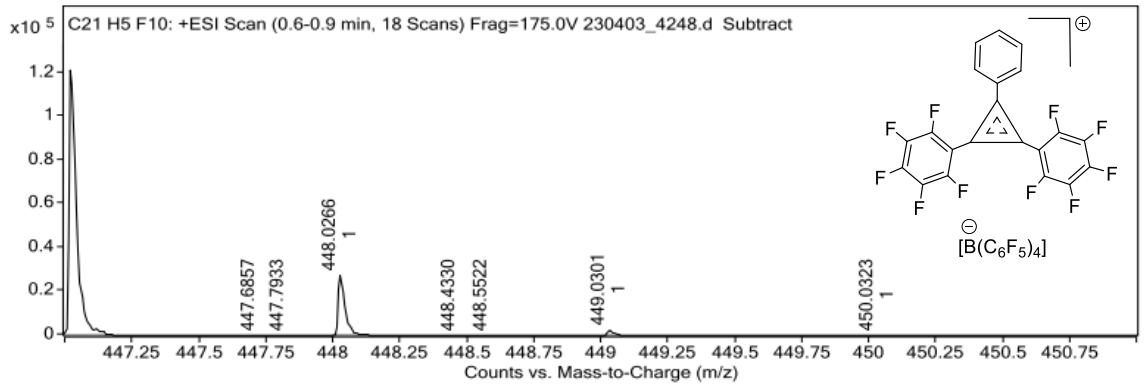
Compound 3

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	447.0236	C21 H5 F10

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
447.0236	C21 H5 F10	447.0226	1.0	2.2	14.5	97.59
447.0236	C9 H9 F10 N2 O7	447.0245	-0.9	-2.0	1.5	79.41
447.0236	C10 H5 F10 N6 O3	447.0258	-2.2	-4.9	6.5	77.30



Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	447.0236	447.0226	1.0	100.0	100.0	0.0
2	448.0266	448.0260	0.6	21.5	22.8	1.3
3	449.0301	449.0293	0.8	2.1	2.5	0.4

Figure S92. HRMS (ESI) spectrum of the compound **3**.

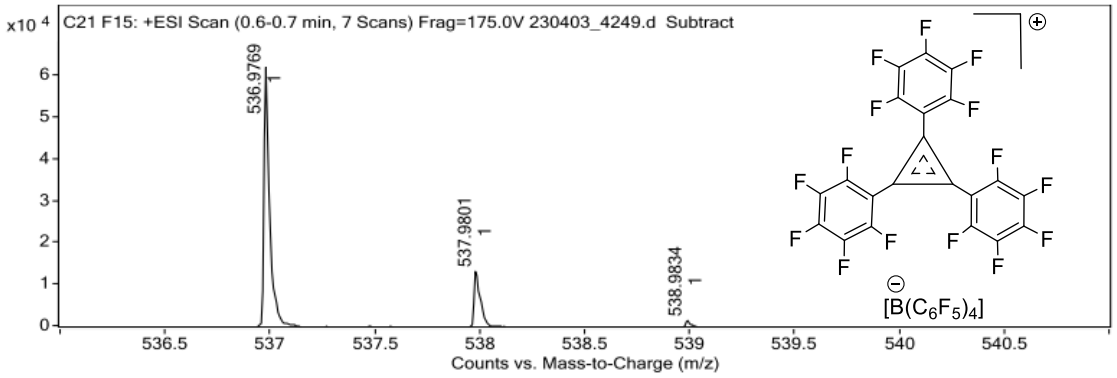
Compound 4a

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	536.9769	C21 F15

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
536.9769	C21 F15	536.9755	1.4	2.6	14.5	96.67
536.9769	C10 F15 N6 O3	536.9787	-1.8	-3.4	6.5	79.19
536.9769	C9 H4 F15 N2 O7	536.9773	-0.4	-0.7	1.5	79.00
536.9769	C14 H4 F15 O5	536.9814	-4.5	-8.4	5.5	63.39



Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	536.9769	536.9755	1.4	100.0	100.0	0.0
2	537.9801	537.9789	1.2	22.5	22.7	0.2
3	538.9834	538.9822	1.2	2.5	2.5	0.0

Figure S93. HRMS (ESI) spectrum of the compound **4a**.

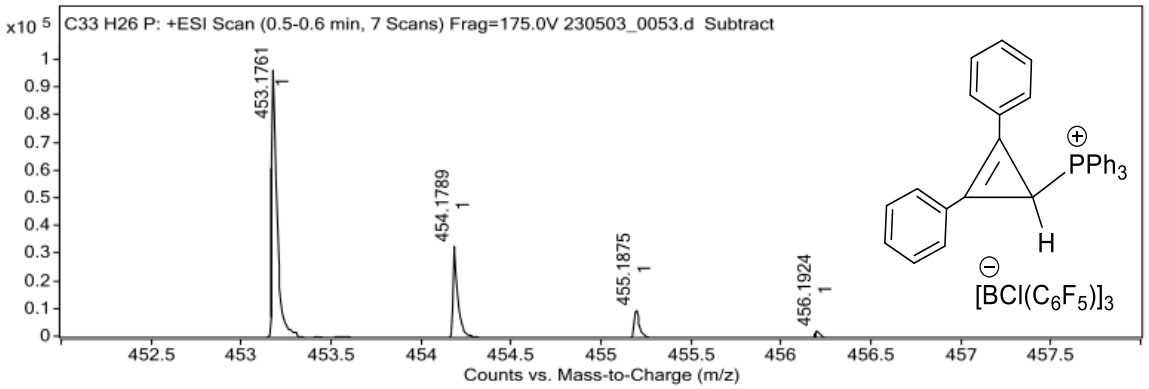
Compound 8

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	453.1761	C33 H26 P

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
453.1761	C33 H26 P	453.1767	-0.6	-1.3	21.5	88.41
453.1761	C23 H25 N4 O6	453.1769	-0.8	-1.8	13.5	81.91
453.1761	C24 H21 N8 O2	453.1782	-2.1	-4.6	18.5	78.81
453.1761	C22 H29 O10	453.1755	0.6	1.3	8.5	76.86
453.1761	C17 H26 N8 O5 P	453.1758	0.3	0.7	9.5	70.65
453.1761	C21 H30 N2 O7 P	453.1785	-2.4	-5.3	8.5	69.38
453.1761	C19 H21 N10 O4	453.1742	1.9	4.2	14.5	63.27
453.1761	C28 H26 N2 O2 P	453.1726	3.5	7.7	17.5	62.87
453.1761	C22 H26 N6 O3 P	453.1799	-3.8	-8.4	13.5	61.60
453.1761	C16 H30 N4 O9 P	453.1745	1.6	3.5	4.5	60.38



Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	453.1761	453.1767	-0.6	100.0	100.0	0.0
2	454.1789	454.1800	-1.1	35.1	36.0	0.9
3	455.1875	455.1834	4.1	10.5	6.3	-4.2
4	456.1924	456.1868	5.6	2.7	0.7	-2.0

Figure S94. HRMS (ESI) spectrum of the compound **8**.

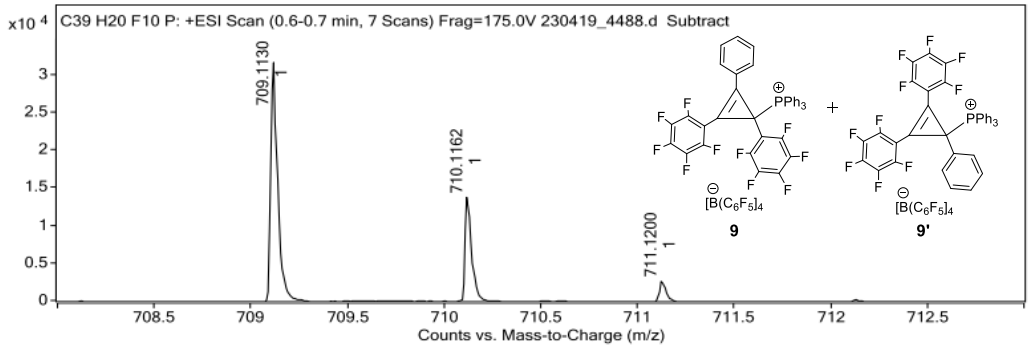
Compound 9 and 9'

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	709.113	C39 H20 F10 P

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
709.1130	C39 H20 F10 P	709.1137	-0.7	-1.0	25.5	98.59
709.1130	C29 H19 F10 N4 O6	709.1139	-0.9	-1.3	17.5	88.07
709.1130	C30 H15 F10 N8 O2	709.1153	-2.3	-3.2	22.5	87.12
709.1130	C28 H23 F10 O10	709.1126	0.4	0.6	12.5	84.77
709.1130	C34 H20 F10 N2 O2 P	709.1097	3.3	4.7	21.5	83.39
709.1130	C25 H15 F10 N10 O4	709.1113	1.7	2.4	18.5	79.53
709.1130	C27 H24 F10 N2 O7 P	709.1156	-2.6	-3.7	12.5	76.50
709.1130	C36 H15 F10 N4 O	709.1081	4.9	6.9	26.5	74.45
709.1130	C28 H20 F10 N6 O3 P	709.1169	-3.9	-5.5	17.5	72.51
709.1130	C34 H19 F10 N2 O4	709.1180	-5.0	-7.1	21.5	72.24

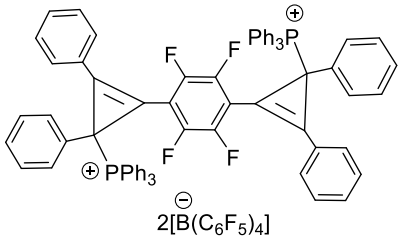


Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	709.1130	709.1137	-0.7	100.0	100.0	0.0
2	710.1162	710.1171	-0.9	43.6	42.4	-1.2
3	711.1200	711.1205	-0.5	9.0	8.8	-0.2

Figure S95. HRMS (ESI, Positive) spectrum of the compounds **9** and **9'**.

Compound 10



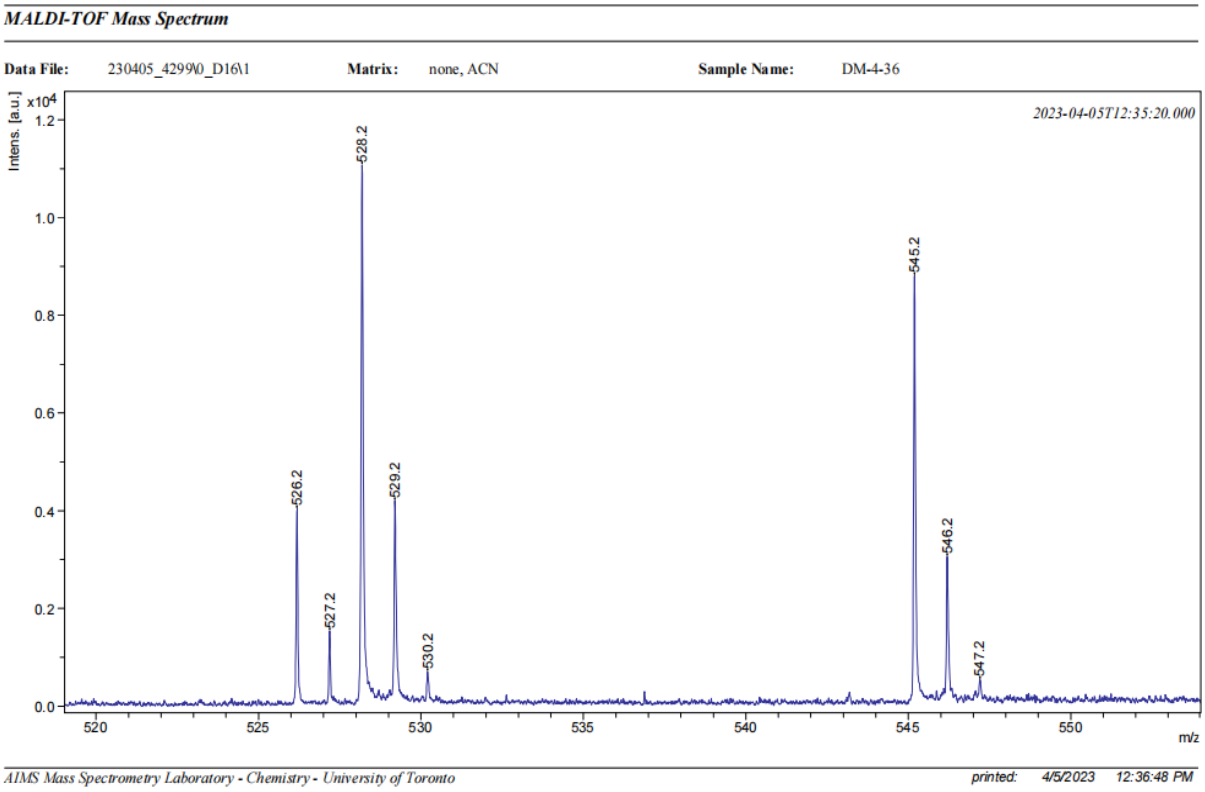


Figure S96. MS (MALDI-TOF) spectrum of the compound **10**.

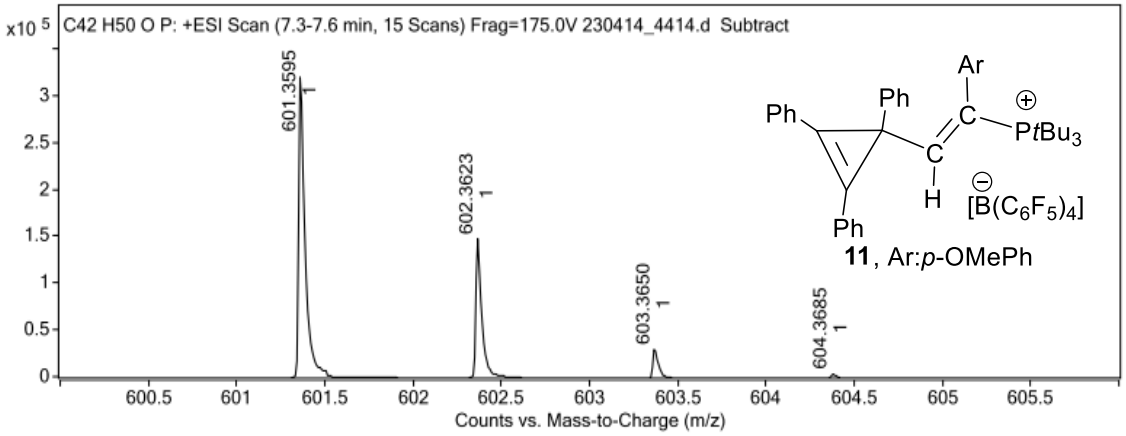
Compound 11

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	601.3595	C42 H50 O P

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
601.3595	C42 H50 O P	601.3594	0.1	0.2	18.5	99.20
601.3595	C44 H45 N2	601.3577	1.8	3.0	23.5	94.39
601.3595	C32 H49 N4 O7	601.3596	-0.1	-0.2	10.5	94.23
601.3595	C33 H45 N8 O3	601.3609	-1.4	-2.3	15.5	93.81
601.3595	C31 H53 O11	601.3582	1.3	2.2	5.5	88.71
601.3595	C26 H50 N8 O6 P	601.3585	1.0	1.7	6.5	85.02
601.3595	C30 H54 N2 O8 P	601.3612	-1.7	-2.8	5.5	84.32
601.3595	C28 H45 N10 O5	601.3569	2.6	4.3	11.5	80.91
601.3595	C31 H50 N6 O4 P	601.3626	-3.1	-5.2	10.5	79.83
601.3595	C37 H50 N2 O3 P	601.3554	4.1	6.8	14.5	78.99

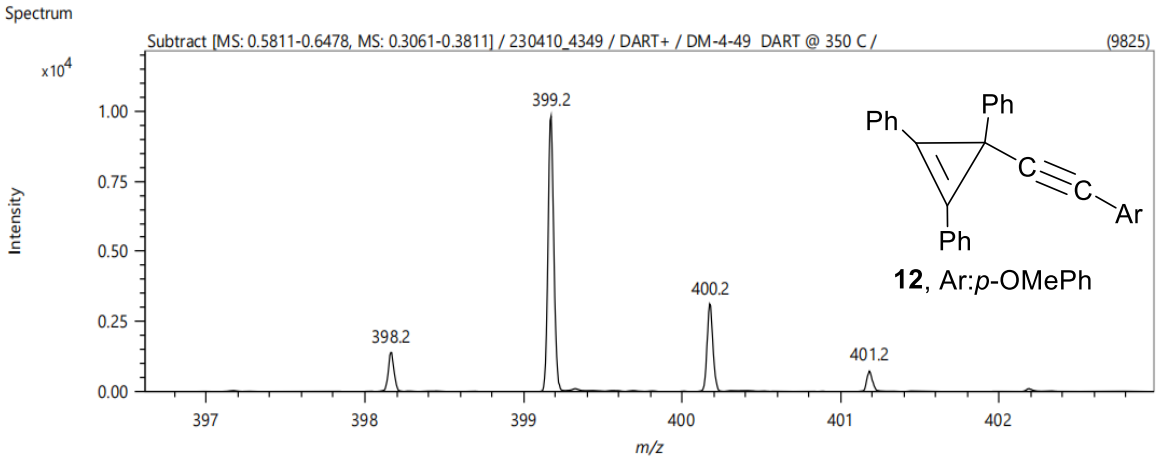


Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	601.3595	601.3594	0.1	100.0	100.0	0.0
2	602.3623	602.3628	-0.5	44.6	46.0	1.4
3	603.3650	603.3661	-1.1	9.8	10.6	0.8
4	604.3685	604.3694	-0.9	1.4	1.6	0.2

Figure S97. HRMS (ESI, Positive) spectrum of the compound **11**.

Compound 12



Elemental Composition

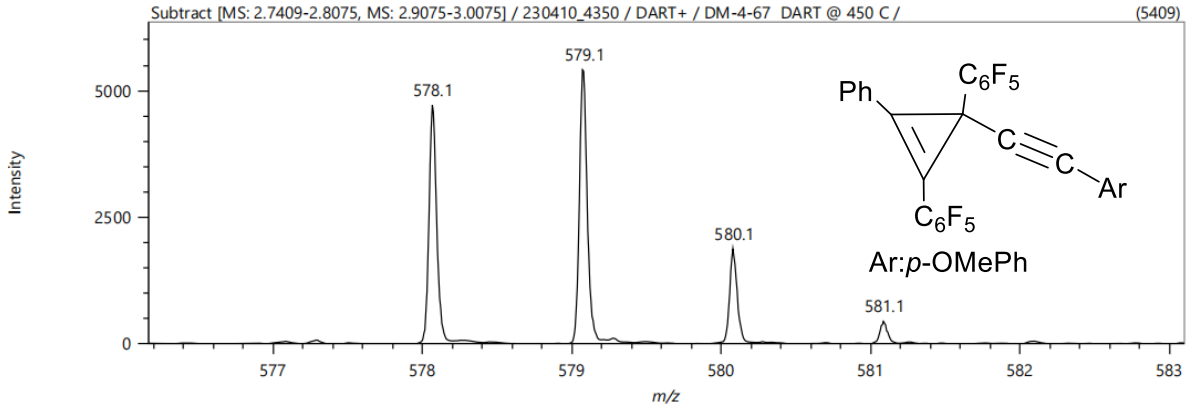
Parameters		Elements Set 2:				
Tolerance:	±10.00 mDa	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	0	0
Charge:	+1	Max	50	100	10	20
DBE:	-1.5 - 100.0					

Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
399.17370	9825.39	C15 H29 N O11	399.17351	0.18	0.46	2.0
		C14 H23 N8 O6	399.17351	0.19	0.48	7.5
		C30 H23 O	399.17434	-0.64	-1.61	19.5
		C28 H21 N3	399.17300	0.70	1.75	20.0
		C16 H25 N5 O7	399.17485	-1.15	-2.89	7.0
		C13 H27 N4 O10	399.17217	1.53	3.83	2.5
		C17 H21 N9 O3	399.17619	-2.49	-6.24	12.0
		C18 H27 N2 O8	399.17619	-2.50	-6.25	6.5
		C11 H25 N7 O9	399.17083	2.87	7.19	3.0
		C25 H23 N2 O3	399.17032	3.38	8.46	15.5
		C19 H23 N6 O4	399.17753	-3.83	-9.60	11.5
		C9 H23 N10 O8	399.16948	4.21	10.55	3.5
		C23 H21 N5 O2	399.16898	4.72	11.83	16.0
		C20 H19 N10	399.17887	-5.17	-12.95	16.5
		C21 H25 N3 O5	399.17887	-5.18	-12.96	11.0
		C8 H27 N6 O12	399.16815	5.55	13.90	-1.5
		C7 H27 N8 O11	399.17938	-5.68	-14.24	-1.5
		C22 H25 N O6	399.16764	6.06	15.18	11.0
		C21 H19 N8 O	399.16763	6.06	15.19	16.5
		C22 H21 N7 O	399.18021	-6.51	-16.32	16.0
		C23 H27 O6	399.18022	-6.52	-16.33	10.5
		C6 H25 N9 O11	399.16680	6.89	17.27	-1.0
		C20 H23 N4 O5	399.16630	7.40	18.54	11.5
		C24 H23 N4 O2	399.18155	-7.86	-19.68	15.5
		C10 H25 N9 O8	399.18206	-8.36	-20.95	3.0
		C19 H27 O9	399.16496	8.74	21.89	6.5
		C18 H21 N7 O4	399.16495	8.74	21.90	12.0
		C26 H25 N O3	399.18290	-9.20	-23.04	15.0
		C12 H27 N6 O9	399.18340	-9.71	-24.31	2.5

Figure S98. HRMS (DART) spectrum of the compound **12.**

Compound 13



Elemental Composition

Parameters		Elements Set 2:					
Tolerance:	±10.00 mDa	Symbol	C	H	N	O	F
Electron:	Odd/Even	Min	0	0	0	0	10
Charge:	+1	Max	50	100	10	20	10
DBE:	-1.5 - 100.0						

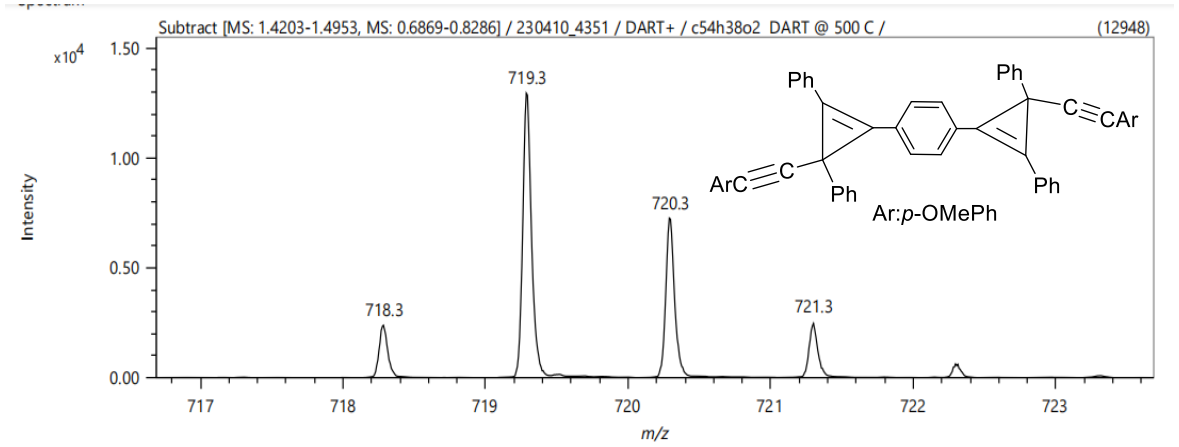
Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
579.07939	5408.88	C15 H19 N O11 F10	579.07929	0.09	0.16	2.0
		C14 H13 N8 O6 F10	579.07929	0.10	0.17	7.5
		C28 H11 N3 F10	579.07878	0.61	1.05	20.0
		C30 H13 O F10	579.08012	-0.74	-1.27	19.5
		C16 H15 N5 O7 F10	579.08063	-1.24	-2.15	7.0
		C13 H17 N4 O10 F10	579.07795	1.44	2.48	2.5

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
		C17 H11 N9 O3 F10	579.08197	-2.58	-4.46	12.0
		C18 H17 N2 O8 F10	579.08197	-2.59	-4.47	6.5
		C11 H15 N7 O9 F10	579.07661	2.78	4.80	3.0
		C25 H13 N2 O3 F10	579.07610	3.29	5.68	15.5
		C19 H13 N6 O4 F10	579.08331	-3.92	-6.78	11.5
		C9 H13 N10 O8 F10	579.07527	4.12	7.12	3.5
		C23 H11 N5 O2 F10	579.07476	4.63	7.99	16.0
		C20 H9 N10 F10	579.08465	-5.26	-9.09	16.5
		C21 H15 N3 O5 F10	579.08465	-5.27	-9.10	11.0
		C8 H17 N6 O12 F10	579.07393	5.46	9.43	-1.5
		C7 H17 N8 O11 F10	579.08516	-5.77	-9.97	-1.5
		C22 H15 N O6 F10	579.07342	5.97	10.30	11.0
		C21 H9 N8 O F10	579.07342	5.97	10.31	16.5
		C22 H11 N7 O F10	579.08599	-6.60	-11.40	16.0
		C23 H17 O6 F10	579.08600	-6.61	-11.41	10.5
		C6 H15 N9 O11 F10	579.07259	6.80	11.75	-1.0
		C20 H13 N4 O5 F10	579.07208	7.31	12.62	11.5
		C24 H13 N4 O2 F10	579.08733	-7.95	-13.72	15.5
		C10 H15 N9 O8 F10	579.08784	-8.45	-14.60	3.0
		C19 H17 O9 F10	579.07074	8.65	14.93	6.5
		C18 H11 N7 O4 F10	579.07074	8.65	14.94	12.0
		C26 H15 N O3 F10	579.08868	-9.29	-16.04	15.0
		C12 H17 N6 O9 F10	579.08918	-9.80	-16.92	2.5
		C17 H15 N3 O8 F10	579.06940	9.99	17.25	7.0
		C16 H9 N10 O3 F10	579.06939	9.99	17.26	12.5

Figure S99. HRMS (DART) spectrum of the compound **13**.

Compound 14



Elemental Composition

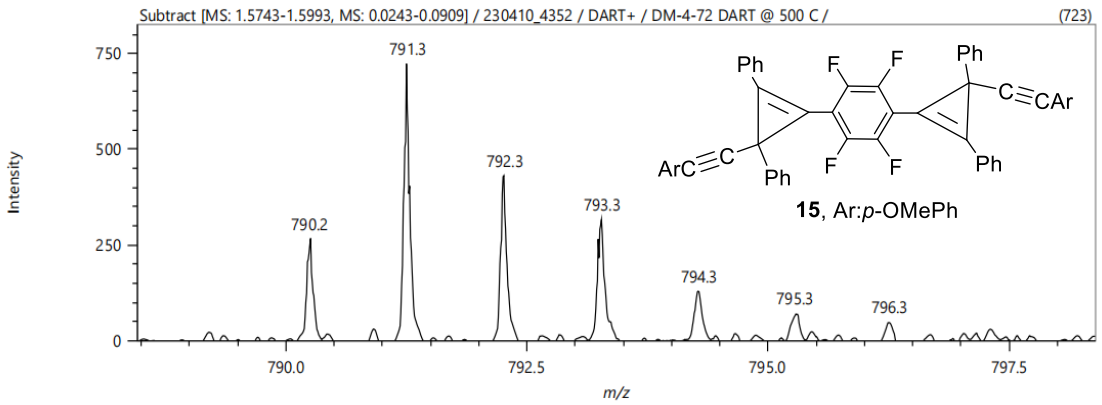
Parameters		Elements Set 2:				
Tolerance:	±10.00 mDa	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	0	0
Charge:	+1	Max	100	200	10	20
DBE:	-1.5 - 100.0					

Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
719.29404	12948.39	C25 H47 N6 O18	719.29414	-0.10	-0.14	5.5
		C39 H45 N O12	719.29363	0.41	0.57	18.0
		C38 H39 N8 O7	719.29362	0.41	0.58	23.5
		C54 H39 O2	719.29446	-0.42	-0.58	35.5
		C52 H37 N3 O	719.29311	0.92	1.28	36.0
		C40 H41 N5 O8	719.29496	-0.93	-1.29	23.0
		C23 H45 N9 O17	719.29279	1.24	1.73	6.0
		C26 H43 N10 O14	719.29547	-1.44	-2.00	10.5
		C27 H49 N3 O19	719.29548	-1.44	-2.00	5.0
		C37 H43 N4 O11	719.29228	1.75	2.44	18.5
		C50 H35 N6	719.29177	2.26	3.15	36.5
		C41 H37 N9 O4	719.29630	-2.27	-3.15	28.0
		C42 H43 N2 O9	719.29631	-2.27	-3.16	22.5
		C28 H45 N7 O15	719.29682	-2.78	-3.86	10.0
		C29 H51 O20	719.29682	-2.78	-3.87	4.5
		C36 H47 O15	719.29095	3.09	4.29	13.5
		C35 H41 N7 O10	719.29094	3.09	4.30	19.0
		C49 H39 N2 O4	719.29043	3.60	5.01	31.5
		C43 H39 N6 O5	719.29764	-3.61	-5.02	27.5
		C20 H47 N8 O20	719.29011	3.92	5.46	1.5
		C30 H47 N4 O16	719.29816	-4.12	-5.73	9.5
		C34 H45 N3 O14	719.28960	4.43	6.16	14.0
		C33 H39 N10 O9	719.28960	4.44	6.17	19.5
		C47 H37 N5 O3	719.28909	4.94	6.87	32.0
		C44 H35 N10 O	719.29898	-4.95	-6.88	32.5
		C45 H41 N3 O6	719.29899	-4.95	-6.88	27.0
		C31 H43 N8 O12	719.29950	-5.46	-7.59	14.5
		C32 H49 N O17	719.29950	-5.46	-7.60	9.0
		C32 H43 N6 O13	719.28826	5.77	8.03	14.5
		C46 H41 N O7	719.28775	6.28	8.73	27.0
		C45 H35 N8 O2	719.28775	6.29	8.74	32.5
		C46 H37 N7 O2	719.30032	-6.29	-8.74	32.0
		C47 H43 O7	719.30033	-6.29	-8.75	26.5
		C33 H45 N5 O13	719.30084	-6.80	-9.46	14.0
		C31 H47 N2 O17	719.28692	7.11	9.89	9.5
		C30 H41 N9 O12	719.28692	7.12	9.89	15.0
		C19 H47 N10 O19	719.30135	-7.31	-10.16	1.5
		C44 H39 N4 O6	719.28641	7.63	10.60	27.5
		C48 H39 N4 O3	719.30167	-7.63	-10.61	31.5

Figure S100. HRMS (DART) spectrum of the compound **14**.

Compound 15



Elemental Composition

Parameters		Elements Set 1:					
Tolerance:	±10.00 mDa	Symbol	C	H	O	N	F
Electron:	Odd/Even	Min	0	0	0	0	4
Charge:	+1	Max	100	200	20	10	4
DBE:	-1.5 - 100.0						

Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
791.25856	723.37	C41 H33 N9 O4 F4	791.25861	-0.05	-0.07	28.0
		C42 H39 N2 O9 F4	791.25862	-0.06	-0.07	22.5
		C28 H41 N7 O15 F4	791.25913	-0.57	-0.72	10.0
		C29 H47 O20 F4	791.25913	-0.57	-0.72	4.5
		C27 H45 N3 O19 F4	791.25779	0.77	0.97	5.0
		C26 H39 N10 O14 F4	791.25779	0.78	0.98	10.5

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
		C40 H37 N5 O8 F4	791.25728	1.28	1.62	23.0
		C43 H35 N6 O5 F4	791.25996	-1.40	-1.76	27.5
		C54 H35 O2 F4	791.25677	1.79	2.26	35.5
		C30 H43 N4 O16 F4	791.26047	-1.91	-2.41	9.5
		C25 H43 N6 O18 F4	791.25645	2.11	2.67	5.5
		C39 H41 N O12 F4	791.25594	2.62	3.31	18.0
		C38 H35 N8 O7 F4	791.25593	2.63	3.32	23.5
		C44 H31 N10 O F4	791.26129	-2.73	-3.45	32.5
		C45 H37 N3 O6 F4	791.26130	-2.74	-3.46	27.0
		C52 H33 N3 O F4	791.25543	3.13	3.96	36.0
		C31 H39 N8 O12 F4	791.26181	-3.25	-4.10	14.5
		C32 H45 N O17 F4	791.26181	-3.25	-4.11	9.0
		C23 H41 N9 O17 F4	791.25511	3.46	4.37	6.0
		C37 H39 N4 O11 F4	791.25460	3.96	5.01	18.5
		C46 H33 N7 O2 F4	791.26264	-4.08	-5.15	32.0
		C47 H39 O7 F4	791.26264	-4.08	-5.16	26.5
		C50 H31 N6 F4	791.25408	4.48	5.66	36.5
		C33 H41 N5 O13 F4	791.26315	-4.59	-5.80	14.0
		C19 H43 N10 O19 F4	791.26366	-5.10	-6.44	1.5
		C36 H43 O15 F4	791.25326	5.30	6.70	13.5
		C35 H37 N7 O10 F4	791.25325	5.31	6.71	19.0
		C48 H35 N4 O3 F4	791.26398	-5.42	-6.85	31.5
		C49 H35 N2 O4 F4	791.25275	5.81	7.35	31.5
		C34 H37 N9 O9 F4	791.26449	-5.93	-7.49	19.0
		C35 H43 N2 O14 F4	791.26449	-5.93	-7.50	13.5
		C20 H43 N8 O20 F4	791.25243	6.14	7.76	1.5
		C21 H45 N7 O20 F4	791.26500	-6.44	-8.14	1.0
		C34 H41 N3 O14 F4	791.25192	6.64	8.40	14.0
		C33 H35 N10 O9 F4	791.25191	6.65	8.40	19.5
		C50 H37 N O4 F4	791.26532	-6.76	-8.55	31.0
		C47 H33 N5 O3 F4	791.25140	7.16	9.05	32.0
		C36 H39 N6 O10 F4	791.26583	-7.27	-9.19	18.5
		C32 H39 N6 O13 F4	791.25057	7.99	10.09	14.5

Figure S101. HRMS (DART) spectrum of the compound **15**.

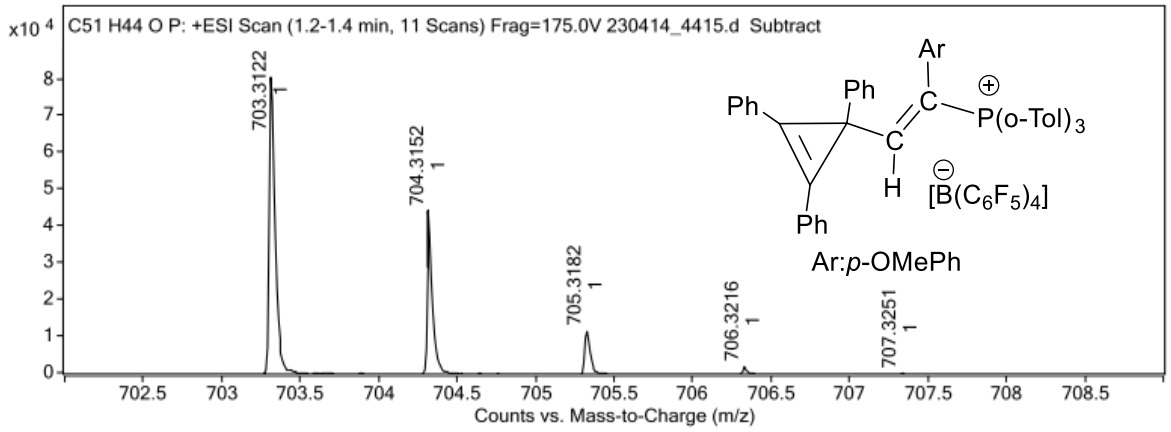
Compound 16

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	703.3122	C51 H44 O P

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
703.3122	C51 H44 O P	703.3124	-0.2	-0.3	30.5	99.27
703.3122	C53 H39 N2	703.3108	1.4	2.0	35.5	96.40
703.3122	C41 H43 N4 O7	703.3126	-0.4	-0.6	22.5	96.17
703.3122	C42 H39 N8 O3	703.3140	-1.8	-2.6	27.5	94.43
703.3122	C40 H47 O11	703.3113	0.9	1.3	17.5	92.98
703.3122	C35 H44 N8 O6 P	703.3116	0.6	0.9	18.5	89.80
703.3122	C39 H48 N2 O8 P	703.3143	-2.1	-3.0	17.5	87.31
703.3122	C37 H39 N10 O5	703.3099	2.3	3.3	23.5	87.15
703.3122	C46 H44 N2 O3 P	703.3084	3.8	5.4	26.5	84.46
703.3122	C40 H44 N6 O4 P	703.3156	-3.4	-4.8	22.5	82.46



Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	703.3122	703.3124	-0.2	100.0	100.0	0.0
2	704.3152	704.3158	-0.6	53.6	55.7	2.1
3	705.3182	705.3192	-1.0	14.3	15.4	1.1
4	706.3216	706.3225	-0.9	2.8	2.8	0.0

Figure S102. HRMS (ESI, Positive) spectrum of the compound **16**.

Experimental references

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Computational details

The quantum chemical DFT calculations have been performed with the TURBOMOLE 7.4 suite of programs[1] The initial structures generated according to their Lewis structures are checked with the CREST method using the xTB program for low-lying conformers as input.[2] The structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO level of theory, which combines the TPSS meta-GGA density functional[3] with the BJ-damped DFT-D3 dispersion correction[4] and the def2-TZVP basis set,[5] using the Conductor-like Screening Model (COSMO) continuum solvation model[6] for CH_2Cl_2 solvent (dielectric constant ε = 8.93 and solvent radium R_{solv} = 2.94 Å). The density-fitting RI-J approach[5a, 7] is used to accelerate the geometry optimization and numerical harmonic frequency calculations[8] in solution. The optimized structures are characterized by frequency analysis to identify the nature of located stationary points (no imaginary frequency for true minima and only one imaginary frequency for transition state) and to provide thermal corrections (at 298.15 K and 1 atm) according to the modified ideal gas–rigid rotor–harmonic oscillator model.[9] This choice of dispersion-corrected meta-GGA functional makes the efficient exploration of all potential reaction paths possible.

The final solvation free energies in CH_2Cl_2 solution are computed with the COSMO-RS solvation model[10] (parameter file: BP_TZVP_C30_1601.ctd) using the COSMOtherm program package[[11] on the above TPSS-D3 optimized structures, and corrected by +1.89 kcal·mol^{-1} to account for higher reference solute concentration of 1 mol·L^{-1} usually used in solution. To check the effects of the chosen DFT functional on the reaction energies and barriers, single-point calculations at the meta-GGA TPSS-D3[3] and hybrid-meta-GGA PW6B95-D3[12] levels are performed using a larger def2-QZVP basis set.[5b, 13] The final reaction Gibbs free energies (ΔG) are determined from the electronic single-point energies plus TPSS-D3 thermal corrections and COSMO-RS solvation free energies. In our discussion, higher-level PW6B95-D3 Gibbs free energies (in kcal/mol, at 298.15 K and 1 mol/L concentration) will be used in our discussion unless specified otherwise. The applied DFT methods in combination with the large AO basis set provide usually accurate electronic energies leading to errors

for chemical energies (including barriers) on the order of typically 1-2 kcal/mol. This has been tested thoroughly for the huge data base GMTKN55[14] which is the common standard in the field of DFT benchmarking.

Table S1. TPSS-D3/def2-TZVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in CH_2Cl_2 solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95-D3); the total PW6B95-D3 free energies G_P; the relative electronic energies (ΔE_T and ΔE_P) and Gibbs energies (ΔG_T and ΔG_P) at the TPSS-D3 and PW6B95-D3 levels. (group Ph = C_6H_5; tBu = CMe_3; To = *o*-$C_6H_5CH_3$)

Reactions in CH_2Cl_2	ImF cm^{-1}	ZPE kcal /mol	Hc kcal /mol	Gc kcal /mol	Hsol kcal /mol	Gsol kcal /mol	TPSS-D3 E_h	PW6B95-D3 E_h	G_P E_h	ΔE_T kcal /mol	ΔE_P kcal /mol	ΔG_P kcal /mol	ΔG_T kcal /mol
*No stable $OPEt_3$ (Et = CH_2CH_3) adduct in CH_2Cl_2 solution with cation **4**$^+$*													
4$^+$ + $OPEt_3$	0	228.66	256.26	171.21	-75.96	-62.22	-2953.37100	-2956.29980	-2956.12009	0.00	0.00	*0.00*	0.00
4$^+$$OPEt_3$	0	229.92	257.73	186.60	-58.14	-51.45	-2953.40144	-2956.33433	-2956.11596	-19.10	-21.67	*2.59*	5.16
Stable BCF (f = C_6F_5) adduct of $OPEt_3$													
Bf_3 + $OPEt_3$	0	219.79	246.70	163.05	-33.59	-22.91	-2864.19373	-2867.03189	-2866.80254	0.00	0.00	*0.00*	0.00
Bf3_OPEt3	0	221.10	248.16	179.22	-24.11	-19.70	-2864.23879	-2867.08293	-2866.82571	-28.27	-32.03	*-14.53*	-10.78
Facile and exergonic Cl- abstraction from 1Cl with BCF													
1Cl + Bf_3	0	224.66	252.42	165.84	-33.81	-25.64	-3248.42315	-3251.64623	-3251.41679	0.00	0.00	*0.00*	0.00
TS0	52i	223.83	252.22	179.10	-29.41	-23.34	-3248.43601	-3251.65931	-3251.40808	-8.07	-8.21	*5.46*	5.60
1$^+$ + $ClBf_3^-$	0	224.25	252.00	165.98	-99.36	-88.69	-3248.32857	-3251.55715	-3251.42796	59.35	55.90	*-7.01*	-3.56
*Facile PPh_3 adduct formation of cation **1+***													
1$^+$ + PPh_3	0	299.14	317.59	250.43	-74.48	-62.13	-1615.12609	-1616.79669	-1616.49060	0.00	0.00	*0.00*	0.00
8$^+$	0	300.11	318.94	265.45	-58.71	-49.66	-1615.19647	-1616.86421	-1616.51733	-44.17	-42.37	*-16.77*	-18.57
*For more delocalized cation **2**$^+$ with 3 phenyl substituents*													
2Cl + Bf_3	0	273.70	304.72	211.54	-38.38	-29.39	-3479.63263	-3483.11243	-3482.81613	0.00	0.00	*0.00*	0.00
TS0a	39i	273.64	305.13	226.42	-32.94	-26.32	-3479.64735	-3483.12867	-3482.80679	-9.23	-10.19	*5.86*	6.82
2$^+$ + $ClBf_3^-$	0	274.19	305.18	212.93	-100.05	-88.40	-3479.56096	-3483.04462	-3482.84015	44.97	42.55	*-15.07*	-12.65
FLP reaction of 2+/PtBu3													
2$^+$ + HCCPhOMe	0	268.05	285.22	221.29	-67.05	-55.48	-1232.73368	-1234.08154	-1233.81127	0.00	0.00	*0.00*	0.00
TS1$^+$	444i	267.27	284.78	233.58	-57.43	-48.62	-1232.73602	-1234.07434	-1233.77658	-1.47	4.52	*21.77*	15.78
A$^+$	0	270.53	287.25	238.15	-60.13	-50.87	-1232.74672	-1234.08646	-1233.78501	-8.18	-3.09	*16.48*	11.39
..followed by facile deprotnation and P-C adduct formation													
2$^+$ + HCCPhOMe + $P(tBu)_3$	0	495.56	524.74	423.56	-80.19	-63.74	-2048.00223	-2050.11247	-2049.53003	0.00	0.00	*0.00*	0.00

TS2^{+}	141i	494.21	524.00	449.80	-61.77	-51.16	-2048.04837	-2050.14498	-2049.50670	-28.96	-20.40	*14.64*	6.08
11 + P(tBu)$_3$H^{+}	0	496.70	525.91	438.23	-83.43	-69.10	-2048.04059	-2050.14921	-2049.55495	-24.07	-23.05	*-15.64*	-16.66
TS3^{+}	93i	496.96	526.20	452.83	-61.46	-51.36	-2048.05265	-2050.15095	-2049.50814	-31.64	-24.14	*13.74*	6.24
10^{+}	0	501.05	529.60	459.19	-63.21	-52.73	-2048.11563	-2050.22217	-2049.57142	-71.16	-68.83	*-25.97*	-28.30
..less Lewis-basic PTo3 leads to higher deprotonation barrier													
2^{+} + HCCPhOMe + P(To)$_3$	0	488.57	519.14	413.23	-88.06	-70.93	-2387.59162	-2390.09659	-2389.54207	0.00	0.00	*0.00*	0.00
TS2+o	294i	486.39	517.74	440.03	-66.89	-55.58	-2387.63150	-2390.12400	-2389.50833	-25.03	-17.20	*21.17*	13.35
11 + P(To)$_3$H^{+}	0	488.85	519.79	426.44	-86.82	-71.04	-2387.61687	-2390.12082	-2389.54845	-15.85	-15.21	*-4.00*	-4.64
*For cation **3**$^{+}$ with 2 Pfs and one Ph, Cl- adduct is 1.6 kcal/mol more stable at C-Pf*													
3Cl + Bf$_3$	0	222.54	259.35	154.50	-34.09	-26.69	-4472.49818	-4476.94755	-4476.73785	0.00	0.00	*0.00*	0.00
3^{+} + ClBf$_3^-$	0	222.71	259.43	154.89	-101.31	-90.83	-4472.40478	-4476.85505	-4476.74694	58.61	58.04	*-5.70*	-5.13
*For cation **4**$^{+}$ with 3 Pfs, Cl- transfer from ClBf$_3^-$ anion is 1.8 kcal/mol endergonic*													
4Cl + Bf$_3$	0	196.74	236.49	125.63	-32.79	-26.05	-4968.92450	-4973.85839	-4973.69367	0.00	0.00	*0.00*	0.00
4^{+} + ClBf$_3^-$	0	196.78	236.47	126.56	-102.05	-92.15	-4968.82428	-4973.75735	-4973.69648	62.89	63.41	*-1.76*	-2.28
*Dication **5**$^{2+}$ formation is also exergonic via two Cl- abstraction*													
5Cl$_2$ + Bf$_3$	0	391.29	431.11	319.94	-55.94	-43.19	-4517.24112	-4521.69382	-4521.24676	0.00	0.00	*0.00*	0.00
5Cl^{+} + Bf$_3$Cl$^-$	0	391.66	431.40	320.11	-112.52	-97.13	-4517.17766	-4521.63382	-4521.27245	39.82	37.65	*-16.12*	-13.94
5Cl^{+} + Bf$_3$	0	391.74	430.42	321.50	-80.23	-66.27	-4056.77566	-4060.89287	-4060.48012	0.00	0.00	*0.00*	0.00
Bf$_3$Cl$^-$ + **5**$^{2+}$	0	393.07	431.45	323.10	-187.73	-170.60	-4056.62142	-4060.74272	-4060.49366	96.79	94.23	*-8.50*	-5.94
*Dication **6**$^{2+}$ formation is also exergonic via two Cl- abstraction*													
6Cl$_2$ + Bf$_3$	0	370.49	412.82	296.91	-54.11	-41.94	-4914.38928	-4919.23071	-4918.81837	0.00	0.00	*0.00*	0.00
6Cl^{+} + ClBf$_3^-$	0	371.57	413.47	298.27	-112.28	-97.28	-4914.31636	-4919.16044	-4918.83412	45.76	44.10	*-9.89*	-8.22
6Cl^{+} + Bf$_3$	0	371.64	412.50	299.66	-79.99	-66.43	-4453.91436	-4458.41950	-4458.04180	0.00	0.00	*0.00*	0.00
6^{2+} + ClBf$_3^-$	0	371.45	412.25	299.64	-186.06	-169.44	-4453.75879	-4458.26687	-4458.05335	97.62	95.78	*-7.25*	-5.40
*In contrast, dication **7**$^{2+}$ formation is somewhat endergonic in solution, but could be favored in solid state*													
7Cl$_2$ + Bf3	0	267.93	321.77	183.19	-45.96	-36.88	-6900.11001	-6906.89039	-6906.65120	0.00	0.00	*0.00*	0.00
7Cl^{+} + Bf$_3$Cl$^-$	0	268.18	321.81	183.40	-112.19	-99.88	-6900.01134	-6906.79016	-6906.65103	61.91	62.89	*0.11*	-0.87
7Cl^{+} + Bf$_3$	0	268.25	320.84	184.79	-79.90	-69.02	-6439.60934	-6446.04922	-6445.85870	0.00	0.00	*0.00*	0.00
Bf$_3$Cl$^-$ + **7**$^{2+}$	0	268.82	321.16	185.35	-190.85	-176.63	-6439.43202	-6445.87102	-6445.85110	111.27	111.82	*4.77*	4.22

Reduction potentials

Fc	0	104.69	110.63	85.30	-11.70	-8.26	-1651.22373	-1652.26457	-1652.13878	0.00	0.00	*0.00*	0.00
Fc^+	0	106.68	112.58	86.28	-53.97	-48.40	-1650.98001	-1652.02772	-1651.96435	152.93	148.63	*109.46*	113.77
2+	0	180.32	191.26	154.54	-54.05	-46.53	-809.53663	-810.42965	-810.25452	0.00	0.00	*0.00*	0.00
2r	0	183.55	193.12	158.39	-23.01	-17.08	-809.70916	-810.59977	-810.37157	-108.26	-106.75	*-73.45*	-74.96
1+	0	130.39	138.08	107.58	-53.35	-46.82	-578.30425	-578.94218	-578.84234	0.00	0.00	*0.00*	0.00
1r	0	131.33	138.46	108.88	-17.51	-12.65	-578.48817	-579.12302	-578.96667	-115.41	-113.48	*-78.02*	-79.95
3+	0	128.85	145.52	96.50	-55.31	-48.96	-1802.38045	-1804.24008	-1804.16131	0.00	0.00	*0.00*	0.00
3r	0	130.81	146.42	99.68	-18.78	-14.57	-1802.57959	-1804.43961	-1804.30097	-124.96	-125.20	*-87.64*	-87.39
4+	0	102.92	122.56	68.17	-56.04	-50.28	-2298.79996	-2301.14237	-2301.11085	0.00	0.00	*0.00*	0.00
4r	0	104.40	122.95	70.50	-17.17	-13.64	-2299.00827	-2301.35236	-2301.25874	-130.72	-131.77	*-92.80*	-91.75
5++	0	299.21	317.53	264.71	-141.73	-128.73	-1386.59710	-1388.12774	-1387.90803	0.00	0.00	*0.00*	0.00
5+r	0	305.92	322.13	274.37	-60.79	-50.26	-1386.88166	-1388.41153	-1388.05138	-178.57	-178.08	*-89.95*	-90.44
5+r	0	305.92	322.13	274.37	-60.79	-50.26	-1386.88166	-1388.41153	-1388.05138	0.00	0.00	*0.00*	0.00
500	0	296.75	315.02	262.65	-39.49	-30.01	-1387.04964	-1388.57859	-1388.20484	-105.41	-104.83	*-96.30*	-96.88
6++	0	277.58	298.34	241.24	-140.06	-127.57	-1783.73446	-1785.65190	-1785.46773	0.00	0.00	*0.00*	0.00
6+r	0	284.25	303.01	250.35	-59.33	-49.34	-1784.03023	-1785.94962	-1785.62628	-185.60	-186.83	*-99.49*	-98.26
6+r	0	284.25	303.01	250.35	-59.33	-49.34	-1784.03023	-1785.94962	-1785.62628	0.00	0.00	*0.00*	0.00
600	0	276.21	296.97	239.71	-35.88	-27.62	-1784.21231	-1786.13337	-1785.79237	-114.26	-115.31	*-104.23*	-103.18
7++	0	174.95	207.25	126.95	-144.85	-134.76	-3769.40769	-3773.25604	-3773.26547	0.00	0.00	*0.00*	0.00
7+r	0	177.59	208.36	132.66	-60.37	-52.76	-3769.72523	-3773.57804	-3773.44770	-199.26	-202.06	*-114.35*	-111.55
7+r	0	177.59	208.36	132.66	-60.37	-52.76	-3769.72523	-3773.57804	-3773.44770	0.00	0.00	*0.00*	0.00
700	0	172.03	204.87	123.89	-29.65	-23.97	-3769.93141	-3773.78871	-3773.62647	-129.38	-132.20	*-112.18*	-109.36

Table S2. TPSS-D3/def2-TZVP + COSMO optimized Cartesian coordinates (in Å) in CH_2Cl_2 solution. Each structure is labeled by a specific name (See Table S1), followed by the number of atoms, the total energy (in hartrees), and the detailed atomic coordinates (in double-column text list).

10$^+$: alkyne FLP adduct of **2**$^+$ / P(*t*Bu)$_3$
94
Energy = -2048.051242735

C	-1.1832792	-1.4282566	-0.3395474
C	-1.5907427	-0.5255047	-1.3311299
C	-1.7515961	-2.7085804	-0.3270645
C	-0.1316265	-1.0401912	0.6633622
H	-1.1521320	0.4686433	-1.3591357
C	-2.5479573	-0.8889215	-2.2764172
H	-1.4292955	-3.4341396	0.4150533
C	-2.7106154	-3.0765208	-1.2720168
C	0.4189121	0.3882265	0.6528589
C	1.1999367	-0.5279873	0.1424945
C	-3.1145787	-2.1663078	-2.2496521
H	-2.8555672	-0.1730349	-3.0336459
H	-3.1359514	-4.0760846	-1.2480636
C	0.0823344	1.7057675	1.0984980
C	2.3568870	-0.9786328	-0.5710282
H	-3.8602132	-2.4497284	-2.9868493
C	-1.2276785	1.9953673	1.5256455
C	1.0587096	2.7216216	1.1419523
C	3.4490428	-0.1195889	-0.7936064
C	2.4137876	-2.3025314	-1.0429329
H	-1.9814636	1.2142307	1.4875306
C	-1.5534169	3.2685589	1.9815969
H	2.0729045	2.5021869	0.8230574
C	0.7265028	3.9909106	1.6033726
H	3.4118811	0.9009605	-0.4268366
C	4.5772059	-0.5842508	-1.4611198
H	1.5683177	-2.9612638	-0.8686772
C	3.5412221	-2.7590919	-1.7164335
C	-0.5783994	4.2692160	2.0236687
H	-2.5675475	3.4831198	2.3054702
H	1.4854794	4.7670339	1.6378792
H	5.4215788	0.0800905	-1.6192658
C	4.6276602	-1.9034319	-1.9220107
H	3.5789399	-3.7825901	-2.0776378
H	-0.8330114	5.2618299	2.3829823
H	5.5102417	-2.2624892	-2.4434738
C	-0.2723587	-1.6611935	2.0081961
C	0.6648722	-1.8423219	2.9689174
H	-1.3017747	-1.9169506	2.2362063
C	2.1082459	-1.5901487	2.7025275
C	2.9115903	-2.6040062	2.1768187
C	2.6915382	-0.3344243	2.9372379
C	4.2668311	-2.4026675	1.9204126
H	2.4746359	-3.5742020	1.9595671
C	4.0341316	-0.1107274	2.6767813
H	2.0753300	0.4842873	3.2970500
C	4.8337517	-1.1494101	2.1713927
H	4.8556912	-3.2110694	1.5050224
H	4.4813312	0.8646760	2.8417425
O	6.1395094	-0.8358517	1.9362363
C	6.9764995	-1.8716316	1.3886437
H	6.5883463	-2.2054616	0.4206603
H	7.9574864	-1.4148672	1.2628027
H	7.0429741	-2.7194485	2.0793595
P	0.0895641	-2.3814371	4.6245646
C	1.5152907	-2.2951481	5.8863177
C	1.8265753	-0.8349845	6.2767439
C	1.1434023	-3.0759273	7.1684249
C	2.8509275	-2.8861749	5.3644387
H	2.0773375	-0.2254595	5.4071122
H	1.0251725	-0.3554955	6.8382069
H	2.7103925	-0.8662045	6.9238161
H	1.1469255	-4.1547764	7.0046262
H	1.9220113	-2.8542909	7.9063950
H	0.1863684	-2.7857252	7.6000162
H	3.4643062	-3.0767395	6.2524957
H	2.7469867	-3.8241909	4.8236777
H	3.3828792	-2.1774239	4.7325504
C	-0.5433873	-4.1665703	4.4739768
C	0.6536953	-5.1316459	4.3584409
C	-1.4211425	-4.5836902	5.6717541
C	-1.3640636	-4.3489010	3.1814721
H	1.3170143	-4.8576525	3.5329042
H	1.2344445	-5.2030070	5.2782326
H	0.2482114	-6.1260579	4.1419645
H	-2.3576645	-4.0251277	5.7126442
H	-1.6752493	-5.6404099	5.5325117
H	-0.9119483	-4.4886516	6.6300218
H	-1.7290984	-5.3815938	3.1812609
H	-2.2325110	-3.6923928	3.1162375
H	-0.7391600	-4.2137199	2.2970623
C	-1.3114909	-1.1943083	5.1515062
C	-2.6528133	-1.4978659	4.4472369
C	-1.5917140	-1.2603345	6.6683165
C	-0.9128927	0.2467275	4.7682605
H	-2.6120646	-1.3709231	3.3645899
H	-3.0440399	-2.4887655	4.6791145
H	-3.3732030	-0.7643523	4.8256884
H	-0.7476122	-0.9309032	7.2731580
H	-2.4241736	-0.5767308	6.8678052
H	-1.8971342	-2.2564000	6.9936556
H	-1.7307600	0.9052241	5.0810400
H	-0.0041050	0.5861494	5.2645403
H	-0.7835599	0.3571955	3.6912230

11 : alkyne deprotonation product
53
Energy = -1232.308989187

C	-2.2327695	-1.5346829	-1.7999371
C	-2.6684351	-1.5996002	-3.1316901
C	-2.8691484	-2.3389338	-0.8466595
C	-1.1040131	-0.6130962	-1.4167883
H	-2.1846125	-0.9818324	-3.8833829
C	-3.7122768	-2.4465411	-3.4984957
H	-2.5380411	-2.2938028	0.1872212
C	-3.9157387	-3.1876066	-1.2129103
C	-0.9242831	0.6900317	-2.1883807
C	-0.0579360	-0.2526432	-2.4655626
C	-4.3424340	-3.2460472	-2.5403825
H	-4.0349413	-2.4833125	-4.5356817
H	-4.3976102	-3.8039147	-0.4583232
C	-1.5270785	1.9822084	-2.3237883
C	1.0592512	-0.8287649	-3.1525118
H	-5.1561838	-3.9063425	-2.8269613
C	-2.6483334	2.3101778	-1.5384448
C	-1.0227881	2.9344368	-3.2323310
C	1.7757381	-0.1018735	-4.1246626
C	1.4502470	-2.1484576	-2.8568853
H	-3.0341788	1.5744913	-0.8391093
C	-3.2501011	3.5592437	-1.6590116
H	-0.1580654	2.6889177	-3.8414494
C	-1.6290660	4.1809049	-3.3473151
H	1.4802252	0.9165705	-4.3581751
C	2.8547031	-0.6856149	-4.7801521
H	0.8964319	-2.7062504	-2.1076479
C	2.5308721	-2.7261692	-3.5169296
C	-2.7434289	4.4976615	-2.5625925
H	-4.1149457	3.8031697	-1.0488324
H	-1.2344732	4.9094808	-4.0498113
H	3.4019003	-0.1186734	-5.5279101
C	3.2358689	-1.9979818	-4.4795318
H	2.8250319	-3.7450385	-3.2821187
H	-3.2138550	5.4721814	-2.6560585
H	4.0789882	-2.4497918	-4.9940106
C	-0.6869713	-0.6345769	-0.0339069
C	-0.3167309	-0.6325216	1.1248279
C	0.1219516	-0.6205794	2.4764919
C	-0.4107379	-1.5155937	3.4217908
C	1.1079779	0.2934034	2.9112172
C	0.0149858	-1.5086849	4.7486605
H	-1.1694190	-2.2275419	3.1112593
C	1.5374605	0.3066250	4.2287888
H	1.5324742	0.9941378	2.1989298
C	0.9943166	-0.5944350	5.1582005
H	-0.4190210	-2.2137548	5.4481107
H	2.2957586	1.0102721	4.5592738
O	1.4800582	-0.5060985	6.4335123
C	0.9430233	-1.4187902	7.4078674
H	1.1464751	-2.4562503	7.1198827
H	1.4568958	-1.1828115	8.3393473
H	-0.1358302	-1.2682010	7.5262763

1Cla : less stable with Cl at CPh
27
Energy = -1038.750355091

H	-0.2926905	-3.0412724	0.7566766
C	-0.0719528	-1.9848641	0.7824468
C	-0.5792966	-0.6657612	1.1743337
C	0.7079403	-0.9590002	0.5220276
C	-1.7232184	0.0390852	0.5075285
C	1.9029829	-0.3502941	0.0006908
C	-1.7112852	0.1150138	-0.8951595
C	-2.8036317	0.5947939	1.2009780
C	2.0505208	1.0463991	0.0580845
C	2.9231385	-1.1349926	-0.5675858
H	-0.8790954	-0.3113374	-1.4483361
C	-2.7537506	0.7313313	-1.5837692
H	-2.8232862	0.5508570	2.2842340
C	-3.8505527	1.2072993	0.5089654
H	1.2604929	1.6454837	0.5007282
C	3.1999025	1.6483897	-0.4467775
H	2.8081317	-2.2142113	-0.6089586
C	4.0683520	-0.5268816	-1.0714185
C	-3.8312525	1.2799838	-0.8840416
H	-2.7217861	0.7847877	-2.6684964
H	-4.6821616	1.6308130	1.0654027
H	3.3104738	2.7276457	-0.4003029
C	4.2087224	0.8639451	-1.0122653
H	4.8546502	-1.1341581	-1.5100506
H	-4.6443845	1.7613058	-1.4198477
H	5.1048883	1.3346061	-1.4060488
Cl	-0.4801296	-0.2521084	3.0097629

1Cl : adduct of $\mathbf{1}^{+}$ and chloride
27
Energy = -1038.764608546

H	0.0617953	-2.7081039	-1.0447656
C	0.0554063	-1.9885904	-0.2315226
C	-0.5858282	-0.6798116	-0.2239116
C	0.7446257	-0.7050425	-0.1910969
C	-1.8551688	-0.0110345	-0.2263444
C	2.0370779	-0.0849200	-0.1302050
C	-3.0382484	-0.7742262	-0.2414299
C	-1.9432038	1.3947455	-0.2129167
C	2.1777399	1.3165477	-0.1115763
C	3.1896195	-0.8925481	-0.0872406
H	-2.9682806	-1.8578924	-0.2450016
C	-4.2793691	-0.1445274	-0.2441871
H	-1.0353764	1.9897350	-0.1996365
C	-3.1865583	2.0176909	-0.2201310
H	1.2936186	1.9456463	-0.1428612
C	3.4427256	1.8917646	-0.0567851
H	3.0787178	-1.9728116	-0.0949361
C	4.4523648	-0.3104344	-0.0281688
C	-4.3568298	1.2510800	-0.2353578

H	-5.1875488	-0.7399760	-0.2533148
H	-3.2471118	3.1020315	-0.2124104
H	3.5439227	2.9730360	-0.0453536
C	4.5822553	1.0812101	-0.0142262
H	5.3365849	-0.9399705	0.0069778
H	-5.3259532	1.7413641	-0.2390705
H	5.5682723	1.5342727	0.0312765
Cl	-0.0035269	-3.0423764	1.3429968

1^{+}P(*t*Bu)$_3$: adduct of **1**$^{+}$ and P(*t*Bu)$_3$

66

Energy = -1393.615924584

H	-0.1389811	-0.4012292	-2.1555163
C	-0.0442426	0.0829272	-1.1783952
C	-0.5709562	1.4901591	-0.9948749
C	0.7333157	1.3759098	-1.0663906
C	-1.7497318	2.3089777	-0.8935022
C	2.0338649	1.9877846	-1.1104800
C	-1.6895617	3.5387575	-0.2084976
C	-2.9681238	1.9137658	-1.4761960
C	3.1370235	1.3348107	-1.6902750
C	2.2123240	3.2777485	-0.5701388
H	-0.7607861	3.8470839	0.2595967
C	-2.8198432	4.3429048	-0.1051966
H	-3.0235688	0.9792980	-2.0231903
C	-4.0922393	2.7280086	-1.3795090
H	3.0071536	0.3536926	-2.1301921
C	4.3832316	1.9535091	-1.7244310
H	1.3699214	3.7908590	-0.1186919
C	3.4615534	3.8873546	-0.6010149
C	-4.0240602	3.9415076	-0.6903545
H	-2.7626693	5.2835930	0.4341499
H	-5.0235236	2.4161267	-1.8425202
H	5.2249856	1.4416467	-2.1810784
C	4.5517632	3.2272261	-1.1759313
H	3.5870774	4.8778589	-0.1742771
H	-4.9045984	4.5716566	-0.6096050
H	5.5267523	3.7045749	-1.1975399
P	-0.0959861	-1.1948691	0.1485116
C	0.6070343	-0.4991088	1.7571846
C	2.1433543	-0.3763789	1.6773175
C	0.0714510	0.9230854	2.0613133
C	0.2496160	-1.4198352	2.9440579
H	2.6450618	-1.3437032	1.6304459
H	2.4647248	0.2406742	0.8353857
H	2.4693213	0.1212734	2.5975240
H	-1.0071721	1.0260928	1.9565621
H	0.3295276	1.1372215	3.1043697
H	0.5561244	1.6718484	1.4353122
H	0.7818832	-1.0348707	3.8208540
H	-0.8169650	-1.4027769	3.1735689
H	0.5624846	-2.4536712	2.7913195
C	0.9507435	-2.6217310	-0.5148622
C	2.2327667	-2.0576528	-1.1624159
C	1.3325514	-3.6380596	0.5789365
C	0.2003776	-3.3694821	-1.6381820
H	1.9932291	-1.4723413	-2.0527409
H	2.8344802	-1.4522471	-0.4868808
H	2.8390594	-2.9128426	-1.4802658
H	0.4615783	-4.0581506	1.0850358
H	1.8633643	-4.4614144	0.0881915
H	2.0046020	-3.2131975	1.3263616
H	0.9127737	-4.0756350	-2.0788797
H	-0.6484835	-3.9458934	-1.2689906
H	-0.1352765	-2.6995692	-2.4342824
C	-1.9027984	-1.7152171	0.3435566
C	-2.6806502	-0.6452029	1.1385415
C	-2.5636168	-1.8136946	-1.0505714
C	-2.0594193	-3.0703433	1.0611611
H	-2.3601864	-0.5776615	2.1787799
H	-2.6191860	0.3420567	0.6757508
H	-3.7336900	-0.9470559	1.1358117
H	-2.2133532	-2.6671821	-1.6278656
H	-3.6398312	-1.9379868	-0.8894761
H	-2.4163665	-0.9086997	-1.6411616
H	-3.1335685	-3.2647378	1.1580132
H	-1.6276734	-3.8948086	0.4911618
H	-1.6295328	-3.0702731	2.0636215

1r : radical from SET reduction of **1**$^{+}$

26

Energy = -578.4638621873

H	-0.8984565	-1.5131274	0.0038169
C	-0.3453359	-0.5832648	0.0009128
C	-0.3825247	0.7848420	0.0032287
C	0.8745897	0.0372434	-0.0062451
C	-1.1143104	1.9879557	0.0119522
C	2.2811054	-0.0314700	-0.0125411
C	-2.5385802	1.9708832	0.0247725
C	-0.4594206	3.2504878	0.0088331
C	3.0780065	1.1466697	-0.0144575
C	2.9459648	-1.2912063	-0.0158232
H	-3.0558151	1.0152272	0.0274845
C	-3.2574406	3.1550670	0.0340856
H	0.6257391	3.2846653	-0.0008734
C	-1.1942060	4.4278569	0.0180801
H	2.5901046	2.1165619	-0.0124919
C	4.4633121	1.0628565	-0.0184654
H	2.3530368	-2.2018625	-0.0146642
C	4.3296694	-1.3577438	-0.0197285
C	-2.5958242	4.3948222	0.0308683
H	-4.3437641	3.1225186	0.0440652
H	-0.6752428	5.3827244	0.0154033
H	5.0547501	1.9746351	-0.0196752
C	5.1033054	-0.1845966	-0.0207804
H	4.8196039	-2.3278956	-0.0218726
H	-3.1656745	5.3190727	0.0383319
H	6.1874929	-0.2442191	-0.0233401

1^{+} : cyclpropeniun cation

26
Energy = -578.3323276692

H	-0.9041095	-1.5228173	0.0073247
C	-0.3517482	-0.5942269	0.0058571
C	-0.3527541	0.7749656	0.0085570
C	0.8516980	0.0587465	-0.0001030
C	-1.0869179	1.9941648	0.0149026
C	2.2735278	-0.0043482	-0.0086944
C	-2.4971036	1.9454051	0.0225648
C	-0.4191554	3.2355147	0.0132545
C	3.0457578	1.1749069	-0.0108476
C	2.9037159	-1.2668012	-0.0149234
H	-3.0007821	0.9838818	0.0233870
C	-3.2240993	3.1272392	0.0286861
H	0.6646769	3.2681602	0.0072019
C	-1.1564891	4.4115156	0.0193030
H	2.5573243	2.1430127	-0.0061820
C	4.4310383	1.0881995	-0.0189942
H	2.2990933	-2.1683019	-0.0132021
C	4.2892188	-1.3416564	-0.0231936
C	-2.5547441	4.3567325	0.0269889
H	-4.3086504	3.0980495	0.0348199
H	-0.6489017	5.3703357	0.0179839
H	5.0314312	1.9918245	-0.0203935
C	5.0502028	-0.1666774	-0.0252488
H	4.7811634	-2.3086520	-0.0280492
H	-3.1274387	5.2791801	0.0317633
H	6.1341305	-0.2296501	-0.0318863

2Cl : adduct of $\mathbf{2}^+$ and chloride
37
Energy = -1269.962386000

C	-1.0024903	-1.7353033	0.6061308
C	-1.0639004	-1.7927243	-0.7970859
C	-1.5733057	-2.7762822	1.3449515
C	-0.3158045	-0.5491723	1.2155790
H	-0.6251567	-0.9918452	-1.3854695
C	-1.6800195	-2.8633435	-1.4395138
H	-1.5351377	-2.7463832	2.4279378
C	-2.1907276	-3.8498121	0.6984702
C	-0.2879305	0.7879219	0.6058519
C	0.8544437	0.1161408	0.6246258
C	-2.2477728	-3.8998953	-0.6938809
H	-1.7166798	-2.8870934	-2.5252042
H	-2.6281114	-4.6485991	1.2912122
C	-1.1209303	1.9074430	0.2744640
C	2.2449550	-0.0736941	0.3292422
H	-2.7288957	-4.7353811	-1.1943660
C	-2.4898250	1.8687650	0.6004135
C	-0.5977686	3.0432191	-0.3735360
C	2.9987973	0.9237711	-0.3191250
C	2.8680032	-1.2829451	0.6914219
H	-2.8891225	0.9928471	1.1027604
C	-3.3163017	2.9421851	0.2827323
H	0.4577327	3.0797027	-0.6250108
C	-1.4298720	4.1121453	-0.6888747
H	2.5242745	1.8594625	-0.5983308
C	4.3442596	0.7103038	-0.5993603
H	2.2845746	-2.0485022	1.1940537
C	4.2148128	-1.4892560	0.4089193
C	-2.7894477	4.0648066	-0.3624521
H	-4.3714412	2.9057392	0.5371151
H	-1.0209668	4.9852052	-1.1889370
H	4.9204781	1.4828829	-1.0999484
C	4.9552359	-0.4949452	-0.2369852
H	4.6892569	-2.4243793	0.6913843
H	-3.4356032	4.9020154	-0.6097488
H	6.0064202	-0.6571463	-0.4567656
Cl	-0.3675458	-0.5837303	3.0990288

$\mathbf{2}^+PPh_3$: adduct of $\mathbf{2}^+$ and PPh_3
70
Energy = -1846.360126204

C	-0.4526712	0.3087047	-1.4042117
C	-0.4729490	1.7065790	-0.8214281
C	0.6693921	1.3212644	-1.3444165
C	-1.1317862	0.0002972	-2.7126993
C	-1.3083965	2.6207196	-0.1016611
C	2.0562924	1.4632956	-1.6703863
C	-2.2067532	0.7928538	-3.1351224
C	-0.6956684	-1.0424970	-3.5372005
C	-0.8485170	3.9127186	0.2206963
C	-2.5842778	2.2182192	0.3323995
C	2.7653084	2.6264469	-1.3071778
C	2.7343149	0.4221752	-2.3325062
C	-2.8450881	0.5340264	-4.3472735
H	-2.5422222	1.6177025	-2.5124039
C	-1.3353795	-1.3064592	-4.7481350
H	0.1584666	-1.6432352	-3.2434374
H	0.1329360	4.2327561	-0.1141225
C	-1.6507207	4.7734200	0.9606315
H	-2.9366328	1.2200683	0.0914495
C	-3.3793537	3.0809901	1.0781291
H	2.2492021	3.4332325	-0.7965154
C	4.1205588	2.7350785	-1.5971914
H	2.1895761	-0.4746733	-2.6083730
C	4.0892392	0.5387914	-2.6199974
C	-2.4162964	-0.5224180	-5.1537276
H	-3.6788732	1.1558063	-4.6597212
H	-0.9828923	-2.1180591	-5.3778705
C	-2.9154399	4.3608768	1.3931508
H	-1.2907343	5.7683260	1.2045988
H	-4.3604178	2.7591820	1.4139346
H	4.6620325	3.6319437	-1.3121332
C	4.7857592	1.6935405	-2.2527398
H	4.6052456	-0.2697665	-3.1286169
H	-2.9155371	-0.7271230	-6.0960367
H	-3.5372950	5.0360177	1.9731757
H	5.8445449	1.7827381	-2.4761626
H	0.1428774	-3.3425808	-1.8877729

C	1.0671998	-3.1214767	-1.3642023
C	1.1090987	-2.0993726	-0.4000235
C	2.2090582	-3.8703043	-1.6343279
P	-0.3485780	-1.0616892	-0.1573369
C	2.2940792	-1.8647696	0.3107523
C	3.3959013	-3.6123217	-0.9439865
H	2.1693403	-4.6592846	-2.3785382
C	-0.2830308	-0.2711310	1.4606547
C	-1.7888002	-2.1322614	-0.2154626
C	3.4326311	-2.6186923	0.0345053
H	2.3308039	-1.1081885	1.0853923
H	4.2853492	-4.1966100	-1.1582879
C	0.7198716	0.6637028	1.7773777
C	-1.3043609	-0.5328960	2.3865859
C	-1.7002005	-3.4237305	0.3304094
C	-3.0133203	-1.6631989	-0.7129579
H	4.3461816	-2.4308687	0.5894609
C	0.6904751	1.3262946	3.0003704
H	1.5077322	0.8938973	1.0694862
C	-1.3237561	0.1357911	3.6085023
H	-2.0858870	-1.2480232	2.1524028
C	-2.8298673	-4.2368492	0.3683791
H	-0.7567328	-3.7881831	0.7240058
C	-4.1373060	-2.4843579	-0.6726523
H	-3.0864062	-0.6743813	-1.1502493
C	-0.3322958	1.0676954	3.9146740
H	1.4650526	2.0492475	3.2358854
H	-2.1178849	-0.0702755	4.3184115
C	-4.0464372	-3.7691657	-0.1339651
H	-2.7592735	-5.2344396	0.7898604
H	-5.0816303	-2.1223098	-1.0661916
H	-0.3548736	1.5920537	4.8649546
H	-4.9240066	-4.4077421	-0.1072486

2^{+}P(*t*Bu)$_3$: adduct of **2**$^{+}$ and P(*t*Bu)$_3$

76

Energy = -1624.796562184

C	-0.0336377	-0.0344592	-1.3339292
C	-0.5845418	1.3578820	-1.0690813
C	0.7227791	1.2627799	-1.0819709
C	-0.0689135	-0.5092543	-2.7844302
C	-1.7872516	2.1443085	-1.0034119
C	1.9946108	1.9365473	-1.0712112
C	1.0507015	-0.2641385	-3.5948290
C	-1.2047589	-1.0468928	-3.4034261
C	-1.8264116	3.2941862	-0.1909530
C	-2.9339742	1.7849965	-1.7350511
C	3.2097571	1.2719981	-1.3217245
C	2.0231254	3.3194887	-0.7970446
C	1.0507507	-0.5737998	-4.9535514
H	1.9350293	0.1885832	-3.1640137
C	-1.2122799	-1.3592899	-4.7634133
H	-2.1034321	-1.2286051	-2.8338328
H	-0.9511616	3.5714527	0.3876925
C	-2.9903903	4.0514203	-0.1027102
H	-2.8987300	0.9228118	-2.3922994
C	-4.0903308	2.5537168	-1.6523840
H	3.2105173	0.2085265	-1.5378499
C	4.4142463	1.9673147	-1.2964880
H	1.0931263	3.8451452	-0.6065563
C	3.2294013	4.0101866	-0.7752748
C	-0.0816384	-1.1324286	-5.5462019
H	1.9380415	-0.3735712	-5.5470668
H	-2.1117669	-1.7749513	-5.2080708
C	-4.1250153	3.6839984	-0.8312656
H	-3.0136279	4.9286251	0.5367503
H	-4.9658789	2.2733865	-2.2300596
H	5.3427682	1.4393858	-1.4890519
C	4.4295550	3.3369647	-1.0224079
H	3.2351188	5.0752277	-0.5643759
H	-0.0862671	-1.3763991	-6.6042065
H	-5.0314256	4.2776192	-0.7617548
H	5.3711036	3.8771107	-1.0016782
H	-2.9330370	-0.8316933	-1.1559004
C	-2.8324909	-1.7783518	-0.6236662
C	-1.9278291	-1.6181752	0.6095852
H	-2.5021000	-2.5600953	-1.3066603
H	-3.8275598	-2.0530660	-0.2576548
P	-0.1177191	-1.2711749	0.1134041
C	-2.5225970	-0.4398812	1.4107324
C	-2.0625181	-2.9095093	1.4462701
C	0.7682234	-0.5314221	1.6382561
C	0.7536046	-2.8663932	-0.4342591
H	-2.0629687	-0.3027437	2.3883670
H	-2.4772539	0.4990617	0.8546268
H	-3.5804571	-0.6745358	1.5736393
H	-3.1122826	-2.9755134	1.7533813
H	-1.8370770	-3.8026386	0.8617372
H	-1.4536104	-2.9131096	2.3485781
C	2.3003160	-0.5686541	1.4790644
C	0.3875006	0.9469259	1.9193304
C	0.4280986	-1.3474414	2.9084882
C	2.0596131	-2.5104647	-1.1771838
C	1.1134056	-3.8006829	0.7396435
C	-0.1346093	-3.6617673	-1.4154436
H	2.7034225	-1.5817623	1.4985038
H	2.6389760	-0.0591338	0.5783687
H	2.7190043	-0.0312147	2.3373424
H	-0.6663371	1.1768259	1.7758639
H	0.6317500	1.1362890	2.9704587
H	0.9778037	1.6324755	1.3133890
H	1.0789061	-0.9629445	3.7014721
H	-0.6013711	-1.2083784	3.2372379
H	0.6293174	-2.4128975	2.8051355
H	1.8684973	-1.9439982	-2.0883198
H	2.7678482	-1.9666520	-0.5534586
H	2.5304857	-3.4564241	-1.4668165
H	0.2481165	-4.0974514	1.3325717
H	1.5408220	-4.7080528	0.2982810
H	1.8691956	-3.3725724	1.3992026

H 0.4639384 -4.5084747 -1.7695299
H -1.0268432 -4.0680503 -0.9371210
H -0.4263034 -3.0728409 -2.2858804

2r : radical from SET reduction of $\mathbf{2}^{+}$
36
Energy = -809.6736523691
C -1.1354242 -1.9066633 0.0015893
C -2.5364818 -1.9025354 -0.1320516
C -0.4634150 -3.1363331 0.1322159
C -0.3977745 -0.6678711 0.0043788
H -3.0611067 -0.9599830 -0.2426668
C -3.2455841 -3.0990941 -0.1371620
H 0.6150830 -3.1476827 0.2442697
C -1.1765451 -4.3306123 0.1322397
C -0.4204821 0.7114638 0.0026549
C 0.8282749 -0.0297904 0.0088999
C -2.5677313 -4.3144923 -0.0036885
H -4.3259837 -3.0866090 -0.2437761
H -0.6501528 -5.2744184 0.2368036
C -1.1170027 1.9368556 -0.0002632
C 2.2362448 -0.0568145 0.0101784
H -3.1230352 -5.2478364 -0.0057217
C -2.5398236 1.9891635 0.0543385
C -0.4143853 3.1741269 -0.0592387
C 2.9898450 1.1511066 0.0678175
C 2.9619578 -1.2826080 -0.0461024
H -3.1048878 1.0647363 0.1121011
C -3.2080657 3.2028159 0.0478938
H 0.6694356 3.1642800 -0.1089534
C -1.0964322 4.3819504 -0.0665767
H 2.4648105 2.0992838 0.1187944
C 4.3765057 1.1275291 0.0712467
H 2.4191091 -2.2203217 -0.1030866
C 4.3472553 -1.2907561 -0.0431442
C -2.4973701 4.4125547 -0.0138925
H -4.2938787 3.2146724 0.0928753
H -0.5356006 5.3116696 -0.1141845
H 4.9261451 2.0640033 0.1181474
C 5.0721364 -0.0891156 0.0158231
H 4.8753704 -2.2396148 -0.0882168
H -3.0270614 5.3602935 -0.0205490
H 6.1577772 -0.1024386 0.0178664

$\mathbf{2}^{+}$: cation
36
Energy = -809.5464204786
C -1.1401946 -1.9166888 0.0003988
C -2.5504067 -1.9046777 -0.0094220
C -0.4568778 -3.1503446 0.0092095
C -0.4096478 -0.6890180 0.0012052
H -3.0835684 -0.9615529 -0.0158381
C -3.2567529 -3.0996653 -0.0105328
H 0.6263526 -3.1688636 0.0166491
C -1.1700505 -4.3412867 0.0080378
C -0.3914319 0.6981494 -0.0033231
C 0.8007959 -0.0111803 0.0070554
C -2.5684936 -4.3172763 -0.0018266
H -4.3416691 -3.0864745 -0.0181210
H -0.6408234 -5.2884653 0.0147043
C -1.0892774 1.9446773 -0.0121601
C 2.2292866 -0.0298860 0.0167519
H -3.1237049 -5.2502907 -0.0027344
C -2.4993244 1.9700366 -0.0214990
C -0.3734840 3.1598381 -0.0115774
C 2.9559246 1.1788565 0.0176341
C 2.9241045 -1.2571606 0.0256860
H -3.0573342 1.0413580 -0.0223412
C -3.1737154 3.1833023 -0.0299408
H 0.7098386 3.1496502 -0.0043356
C -1.0548161 4.3692362 -0.0200352
H 2.4303397 2.1261565 0.0104905
C 4.3438425 1.1567698 0.0273126
H 2.3739801 -2.1904915 0.0252620
C 4.3121265 -1.2712577 0.0354062
C -2.4533991 4.3822692 -0.0292138
H -4.2586035 3.1988622 -0.0371082
H -0.5006361 5.3020674 -0.0194947
H 4.8995033 2.0887184 0.0278787
C 5.0223340 -0.0662904 0.0362220
H 4.8432499 -2.2173703 0.0424414
H -2.9836632 5.3296534 -0.0358482
H 6.1079225 -0.0804457 0.0438662

3Cla : higher **3**Cl
37
Energy = -2262.776645230
F 3.0700199 1.7158879 -0.2278699
C 3.1263179 0.3920245 -0.0159816
C 4.3523475 -0.1720358 0.3091131
C 1.9543508 -0.3789656 -0.1124186
F 5.4502433 0.5920127 0.4111720
C 4.4396018 -1.5449852 0.5329785
C 0.7081837 0.2176735 -0.4820790
C 2.0829739 -1.7620980 0.1074881
F 5.6167791 -2.0983925 0.8426417
C 3.3016069 -2.3440456 0.4263038
C -0.6085270 0.2075848 -0.6048395
C 0.1024649 1.3681058 -1.1798633
F 1.0141879 -2.5608516 -0.0339275
F 3.3970752 -3.6683758 0.6202579
C -1.9093450 -0.3191666 -0.3296582
C -0.0100762 2.7414750 -0.5897595
C -3.0306877 0.0949894 -1.0696756
C -2.1396485 -1.2233187 0.7221972
C 0.1701116 2.8774998 0.7952564
C -0.3333643 3.8724040 -1.3452036
F -2.8783790 0.9684361 -2.0766254
C -4.3054551 -0.3855171 -0.8011296
F -1.1192855 -1.6035724 1.5071442

C	-3.4078500	-1.7071122	1.0104345
H	0.4159831	2.0054610	1.3950613
C	0.0362372	4.1203191	1.4091327
C	-0.4720798	5.1164274	-0.7275957
H	-0.4730040	3.7797713	-2.4164898
C	-4.4943029	-1.2914127	0.2411643
F	-5.3541400	0.0145669	-1.5357681
F	-3.5993128	-2.5596115	2.0287399
H	0.1866126	4.2080768	2.4814037
C	-0.2869541	5.2466687	0.6490511
H	-0.7239522	5.9857200	-1.3284614
F	-5.7191642	-1.7554749	0.5099467
H	-0.3913425	6.2167117	1.1264421
Cl	0.3150796	1.3788703	-3.0159026

3Cl : adduct of $\mathbf{3}^+$ and chloride

37

Energy = -2262.779150885

F	3.2692018	0.9011266	-1.5085405
C	2.9908259	-0.0872364	-0.6352764
C	4.0679491	-0.7380634	-0.0457981
C	1.6611027	-0.4232710	-0.3548561
F	5.3276317	-0.3805674	-0.3462592
C	3.8370778	-1.7625670	0.8682208
C	0.5142691	0.3052840	-0.9834151
C	1.4697374	-1.4572340	0.5662837
F	4.8667961	-2.3940209	1.4485095
C	2.5299565	-2.1216243	1.1766743
C	-0.8234853	0.4514726	-0.4087851
C	-0.0858558	1.5535185	-0.4780109
F	0.2253703	-1.8479133	0.9090027
F	2.2953069	-3.1071953	2.0591688
C	-2.0488841	-0.2362773	-0.1307238
C	0.1210357	2.9674007	-0.3460516
C	-3.0255192	0.3021551	0.7230473
C	-2.3278629	-1.4954167	-0.6910591
C	-0.9123447	3.8118385	0.1070637
C	1.3668030	3.5256697	-0.6907491
F	-2.8025958	1.4838004	1.3262506
C	-4.2147175	-0.3573308	0.9982636
F	-1.4408757	-2.0729449	-1.5154754
C	-3.5145671	-2.1687022	-0.4327700
H	-1.8786835	3.3903758	0.3567841
C	-0.6935314	5.1795793	0.2226354
C	1.5766984	4.8957926	-0.5728528
H	2.1569300	2.8792216	-1.0544849
C	-4.4625595	-1.5986092	0.4147007
F	-5.1205438	0.1847483	1.8270386
F	-3.7556369	-3.3630853	-0.9952243
H	-1.4938955	5.8252694	0.5712105
C	0.5500102	5.7247829	-0.1135828
H	2.5400080	5.3191540	-0.8405555
F	-5.6067355	-2.2426748	0.6712356
H	0.7153687	6.7942472	-0.0227806
Cl	0.6095207	0.1050476	-2.8461590

3r : radical from SET reduction of $\mathbf{3}^+$

36

Energy = -1802.495648801

F	3.0792178	1.6059339	0.8378173
C	3.1472055	0.3438796	0.3631635
C	4.3796436	-0.2811154	0.3356175
C	1.9495470	-0.3045856	-0.0358461
F	5.4836105	0.3660704	0.7548846
C	4.4810457	-1.6045400	-0.1029776
C	0.7009407	0.3407021	0.0005428
C	2.1019539	-1.6426318	-0.4860018
F	5.6754976	-2.2197008	-0.1308301
C	3.3300884	-2.2794284	-0.5168880
C	-0.7426803	0.2928168	0.0204839
C	-0.0599946	1.4920180	0.0185188
F	1.0316472	-2.3004235	-0.9722549
F	3.4319925	-3.5399678	-0.9790735
C	-1.9457966	-0.4344076	0.0483238
C	-0.1087757	2.9299943	0.0297259
C	-3.1834159	0.1359076	-0.3477119
C	-2.0086809	-1.7835450	0.4862314
C	-1.2909916	3.5937517	0.4080890
C	1.0250545	3.6792591	-0.3367603
F	-3.1995779	1.4034033	-0.8124012
C	-4.3711891	-0.5706144	-0.3278709
F	-0.8971197	-2.3717554	0.9690798
C	-3.1913583	-2.5016258	0.5093796
H	-2.1615159	3.0156049	0.6949657
C	-1.3313152	4.9834596	0.4274873
C	0.9707655	5.0686291	-0.3309924
H	1.9325829	3.1669899	-0.6338833
C	-4.3843571	-1.9015064	0.0993374
F	-5.5155414	0.0044915	-0.7438398
F	-3.2090140	-3.7700606	0.9607648
H	-2.2403929	5.4936944	0.7303682
C	-0.2038661	5.7215102	0.0547372
H	1.8428916	5.6448504	-0.6240268
F	-5.5354760	-2.5946351	0.1205220
H	-0.2407154	6.8068952	0.0647496

$\mathbf{3}^+$: cation

36

Energy = -1802.347854171

F	3.0539657	1.5024752	0.9722334
C	3.0935765	0.2817228	0.4265751
C	4.3025888	-0.3939318	0.3848919
C	1.9050904	-0.3055711	-0.0482616
F	5.4158002	0.1649854	0.8658329
C	4.3484423	-1.6794544	-0.1601997
C	0.6645519	0.3891890	-0.0015606
C	1.9869703	-1.6030377	-0.5930289
F	5.5049973	-2.3305290	-0.2112069
C	3.1913939	-2.2852056	-0.6571193
C	-0.7118423	0.3438695	0.0223033

C	-0.0630883	1.5722635	0.0183211
F	0.8962083	-2.1694799	-1.1189185
F	3.2591601	-3.5034497	-1.1998376
C	-1.9040996	-0.4311247	0.0617598
C	-0.1090000	2.9919011	0.0276886
C	-3.1305797	0.0848838	-0.3991146
C	-1.8994158	-1.7390344	0.5874988
C	-1.3302223	3.6551676	0.2783211
C	1.0670425	3.7354896	-0.2135988
F	-3.1729683	1.3135959	-0.9264866
C	-4.2934908	-0.6675483	-0.3615822
F	-0.7721267	-2.2417504	1.1008013
C	-3.0570254	-2.4983239	0.6465951
H	-2.2271253	3.0792086	0.4728381
C	-1.3660745	5.0415190	0.2929556
C	1.0138826	5.1213619	-0.2095342
H	1.9989790	3.2209002	-0.4152571
C	-4.2535393	-1.9611996	0.1645023
F	-5.4429949	-0.1739031	-0.8282595
F	-3.0430622	-3.7260714	1.1716802
H	-2.2988030	5.5575013	0.4944799
C	-0.1982650	5.7726450	0.0465449
H	1.9113936	5.6988279	-0.4041065
F	-5.3653715	-2.6863205	0.2114280
H	-0.2330384	6.8577463	0.0542526

4Cl : adduct of $\mathbf{4}^+$ and chloride

37

Energy = -2759.181507321

F	2.0983172	-2.8704886	-1.0059119
C	2.6203785	-1.9047030	-0.2282186
C	2.0307372	-0.6346247	-0.1955070
C	3.7371962	-2.2275109	0.5342856
C	0.8044013	-0.3300180	-0.9994196
C	2.5993377	0.2895041	0.6864618
F	4.2748339	-3.4562832	0.4668952
C	4.2901717	-1.2742613	1.3850938
C	-0.5546569	-0.5342637	-0.4511467
C	-0.1812548	0.7135417	-0.6827043
F	2.0624752	1.5174248	0.8326094
C	3.7129167	-0.0116435	1.4660006
F	5.3617685	-1.5758708	2.1301188
C	-1.4732446	-1.5204748	0.0424347
C	-0.4627629	2.1063408	-0.8338761
F	4.2282303	0.9092792	2.2969983
C	-2.2633932	-1.2819677	1.1800142
C	-1.5792368	-2.7880171	-0.5532338
C	0.4943539	2.9946726	-1.3597541
C	-1.7298111	2.6397614	-0.5355915
F	-2.1562839	-0.1151122	1.8346613
C	-3.1219038	-2.2463010	1.6911590
F	-0.8562856	-3.0698963	-1.6470950
C	-2.4402678	-3.7604256	-0.0609520
F	1.7054939	2.5464153	-1.7185819
C	0.2170791	4.3423417	-1.5452397
F	-2.7001065	1.8309928	-0.0858951
C	-2.0226026	3.9836888	-0.7131276
F	-3.8495835	-1.9966854	2.7900169
C	-3.2150238	-3.4883362	1.0651406
F	-2.5357811	-4.9537956	-0.6654584
F	1.1484671	5.1665502	-2.0462125
C	-1.0427153	4.8395048	-1.2158332
F	-3.2390916	4.4636184	-0.4170107
F	-4.0429809	-4.4201097	1.5489504
F	-1.3163733	6.1347817	-1.3935245
Cl	1.1023111	-0.6335095	-2.7941633

$\mathbf{4}^+OPEt_3$: unstable adduct of $\mathbf{4}^+$ and $OPEt_3$

59

Energy = -2953.310551070

F	-2.4642959	0.9393179	-1.7331834
C	-1.4076860	1.7017577	-2.0762730
C	-0.2343993	1.6628297	-1.3200950
C	-1.5409059	2.5130753	-3.1997182
C	-0.0789509	0.7703272	-0.1291846
C	0.8072012	2.4941760	-1.7423503
F	-2.6844133	2.5187114	-3.8980096
C	-0.4822148	3.3269474	-3.5904088
C	-0.9124986	-0.3890120	0.1989949
C	0.3345082	-0.6464990	-0.1640439
F	1.9734802	2.5118294	-1.0599608
C	0.7009445	3.3198839	-2.8538842
F	-0.5981599	4.1123079	-4.6653051
C	-2.2118170	-0.8114931	0.6207368
C	1.3878801	-1.5907892	-0.4094260
F	1.7267108	4.0993542	-3.2241413
C	-2.6590906	-2.1289819	0.4224919
C	-3.1040832	0.0894599	1.2266124
C	1.4594413	-2.8020715	0.3009139
C	2.4025290	-1.3365774	-1.3455082
F	-1.8670867	-3.0092373	-0.2052037
C	-3.9243601	-2.5366869	0.8208224
F	-2.7238642	1.3607699	1.4304715
C	-4.3696123	-0.3017180	1.6393167
F	0.5510778	-3.0699090	1.2514890
C	2.4804855	-3.7178153	0.0848863
F	2.3763984	-0.1968242	-2.0539086
C	3.4291576	-2.2410732	-1.5801236
F	-4.3348622	-3.7928020	0.6110745
C	-4.7791030	-1.6203345	1.4356588
F	-5.1967100	0.5708797	2.2276574
F	2.5307221	-4.8584103	0.7820416
C	3.4655099	-3.4376937	-0.8632385
F	4.3704311	-1.9807486	-2.4938131
F	-5.9947645	-2.0045446	1.8240404
F	4.4432601	-4.3157223	-1.0843307
P	1.4497763	1.6778350	2.0846241
O	0.2823330	1.6612294	1.0118011
C	2.8845903	0.6978555	1.5910705
C	4.0579668	0.8449592	2.5783391

H	3.1693556	1.0225257	0.5854380
H	2.5663320	-0.3467205	1.5295434
H	4.8846197	0.2177367	2.2363768
H	4.4141235	1.8764563	2.6262818
H	3.7813107	0.5198586	3.5846750
C	1.9097340	3.4124578	2.2484786
C	0.7048482	4.3437810	2.4637213
H	2.4568637	3.6758290	1.3364285
H	2.6138289	3.4763000	3.0858316
H	1.0631576	5.3737030	2.5293977
H	0.0004882	4.2736929	1.6315827
H	0.1765300	4.1090161	3.3915287
C	0.7984819	1.0640465	3.6507754
C	0.4195420	-0.4233923	3.6342359
H	-0.0686596	1.6905620	3.8883139
H	1.5600450	1.2718909	4.4117833
H	0.0031781	-0.6985234	4.6056995
H	-0.3342280	-0.6355835	2.8718061
H	1.2887309	-1.0603953	3.4499800

4r : radical from SET reduction of **4**$^{+}$
36
Energy = -2298.899996459

F	1.4958064	-2.7445378	-0.8824048
C	2.4983204	-1.9566791	-0.4441098
C	2.1967999	-0.6342881	-0.0229763
C	3.7895106	-2.4469229	-0.4807048
C	0.8731438	-0.1702588	0.0111792
C	3.3067212	0.1605714	0.3617050
F	4.0355746	-3.6965478	-0.9140811
C	4.8554743	-1.6290659	-0.0923084
C	-0.4692202	-0.4592316	-0.0009861
C	-0.1394473	0.8751751	0.0091231
F	3.0963815	1.4034914	0.8315358
C	4.6039100	-0.3208540	0.3284486
F	6.1119410	-2.1004778	-0.1191720
C	-1.4988286	-1.4627357	-0.0141850
C	-0.5593208	2.2124382	0.0530619
F	5.6279396	0.4543508	0.7282963
C	-2.6949466	-1.2690407	-0.7223892
C	-1.3416840	-2.6722704	0.6802762
C	0.2806677	3.2997514	-0.3005414
C	-1.8788892	2.5543734	0.4526579
F	-2.8708230	-0.1503501	-1.4396980
C	-3.6892672	-2.2377925	-0.7477333
F	-0.2369273	-2.8825720	1.4099115
C	-2.3322216	-3.6450812	0.6788802
F	1.5250071	3.0523186	-0.7487205
C	-0.1562752	4.6121932	-0.2584972
F	-2.7095691	1.5737847	0.8610738
C	-2.3247518	3.8612011	0.4977521
F	-4.8129916	-2.0461613	-1.4517891
C	-3.5065856	-3.4264264	-0.0411900
F	-2.1750481	-4.7822572	1.3697317
F	0.6616051	5.6140331	-0.6290509
C	-1.4631805	4.9034632	0.1404310
F	-3.5736274	4.1449805	0.9101771
F	-4.4607605	-4.3598168	-0.0542032
F	-1.8917321	6.1751828	0.1760264

4^{+} : cation
36
Energy = -2298.745448937

F	1.6267227	-2.6656861	-1.0583308
C	2.5363588	-1.8583958	-0.5068329
C	2.1352716	-0.6110839	0.0151009
C	3.8680244	-2.2392629	-0.5175664
C	0.7712741	-0.2228327	0.0110972
C	3.1315654	0.2390266	0.5382872
F	4.2413888	-3.4084530	-1.0407977
C	4.8301967	-1.3756597	0.0144865
C	-0.5704777	-0.5606920	-0.0001042
C	-0.1924787	0.7702942	0.0112315
F	2.7814987	1.4029259	1.0915373
C	4.4648731	-0.1359577	0.5478237
F	6.1064902	-1.7373309	0.0135567
C	-1.5872382	-1.5493270	-0.0143487
C	-0.5381741	2.1456323	0.0181726
F	5.3968055	0.6628296	1.0709096
C	-2.8657166	-1.2698299	-0.5399502
C	-1.3488916	-2.8424977	0.4954176
C	0.3506635	3.1202551	-0.4808978
C	-1.7804209	2.5800241	0.5252458
F	-3.1097169	-0.0729081	-1.0795021
C	-3.8591683	-2.2346971	-0.5664229
F	-0.1678154	-3.1246291	1.0511059
C	-2.3383253	-3.8117178	0.4897589
F	1.5117459	2.7396256	-1.0197419
C	0.0174525	4.4646197	-0.4819781
F	-2.6241419	1.6903564	1.0541974
C	-2.1199841	3.9227505	0.5442198
F	-5.0561039	-1.9704557	-1.0933743
C	-3.5925239	-3.5048307	-0.0464958
F	-2.1127641	-5.0232397	1.0011532
F	0.8527344	5.3763972	-0.9830342
C	-1.2186510	4.8628925	0.0358721
F	-3.2852046	4.3271007	1.0530783
F	-4.5420057	-4.4310257	-0.0620156
F	-1.5405575	6.1497235	0.0446680

500 : SET reduction of **5r**$^{+}$
60
Energy = -1386.990154384

H	0.3682698	-2.4236909	-0.4314210
C	0.2118746	-1.3643276	-0.2488185
C	1.2427868	-0.6122655	0.2196877
C	-1.1025342	-0.8042160	-0.5023072
H	2.2036773	-1.0847001	0.4027952
C	1.1026863	0.8045593	0.5000749
C	-1.2425484	0.6126591	-0.2220753

C	-2.1405477	-1.5615384	-0.9742183
C	2.1405204	1.5617224	0.9726086
C	-0.2116343	1.3647537	0.2463787
H	-2.2034790	1.0850472	-0.4050522
C	-2.6925058	-2.8024730	-1.4282690
C	-3.5017659	-1.7168210	-1.3910411
C	2.6922063	2.8023267	1.4278944
C	3.5015878	1.7168269	1.3899505
H	-0.3679923	2.4241629	0.4287937
C	-2.5025485	-4.1947007	-1.7086878
C	-4.7881783	-1.1249248	-1.6096716
C	2.5023704	4.1943727	1.7092677
C	4.7879940	1.1250279	1.6089044
C	-1.2188414	-4.7707920	-1.6008929
C	-3.5833004	-5.0181240	-2.0935185
C	-5.8413784	-1.8590040	-2.1979201
C	-5.0237707	0.2160614	-1.2386620
C	1.2181703	4.7700002	1.6051101
C	3.5839348	5.0180144	2.0913277
C	5.8389908	1.8574206	2.2031494
C	5.0256818	-0.2140271	1.2323605
H	-0.3798075	-4.1475767	-1.3111056
C	-1.0239955	-6.1206346	-1.8738210
H	-4.5789222	-4.5948000	-2.1696742
C	-3.3831927	-6.3666593	-2.3597797
H	-5.6745426	-2.8871267	-2.5001599
C	-7.0821847	-1.2701342	-2.4053498
H	-4.2242840	0.7887168	-0.7812291
C	-6.2699832	0.7984491	-1.4442304
H	0.3786058	4.1465058	1.3174483
C	1.0235968	6.1196651	1.8791450
H	4.5799453	4.5949670	2.1641184
C	3.3840942	6.3664003	2.3585441
H	5.6700995	2.8838121	2.5101601
C	7.0798280	1.2687506	2.4109764
H	4.2277953	-0.7852564	0.7703624
C	6.2720245	-0.7960923	1.4381002
H	-0.0295468	-6.5491126	-1.7897293
C	-2.1032235	-6.9241628	-2.2530594
H	-4.2244889	-6.9886051	-2.6513001
H	-7.8818127	-1.8458752	-2.8621973
C	-7.3033635	0.0600707	-2.0282843
H	-6.4372238	1.8306036	-1.1504990
H	0.0287933	6.5478648	1.7979028
C	2.1035857	6.9234161	2.2557501
H	4.2260022	6.9886304	2.6476839
H	7.8777165	1.8430247	2.8726870
C	7.3032362	-0.0594330	2.0281347
H	6.4410641	-1.8266674	1.1398920
H	-1.9500191	-7.9784980	-2.4635475
H	-8.2752508	0.5167980	-2.1902126
H	1.9505472	7.9775725	2.4672515
H	8.2751815	-0.5159619	2.1902749

5Cl_2a : higher **5**Cl_2

62

Energy = -2307.533625073

H	1.2523192	-2.0057421	0.7566870
C	0.6984113	-1.1326290	0.4262810
C	-0.6687374	-1.2079831	0.2221334
C	1.3892655	0.0781691	0.2098596
H	-1.1911041	-2.1441057	0.3905123
C	-1.3882724	-0.0723812	-0.2036310
C	0.6697748	1.2137450	-0.2160741
C	2.8030884	0.1273732	0.4256604
C	-2.8021043	-0.1215109	-0.4195759
C	-0.6974206	1.1384698	-0.4199099
H	1.1922380	2.1498144	-0.3844061
C	3.9591742	-0.6804700	0.8295351
C	3.9804584	0.7411953	0.4515793
C	-3.9587283	0.6861086	-0.8214659
C	-3.9785545	-0.7371553	-0.4502313
H	-1.2513431	2.0116289	-0.7501789
C	4.5618189	-1.7801442	0.0088817
C	4.8569337	1.8600261	0.2747416
C	-4.5647840	1.7818620	0.0016938
C	-4.8529894	-1.8588839	-0.2820623
C	4.1002374	-1.9464404	-1.3054587
C	5.5928673	-2.6045155	0.4723089
C	6.2326098	1.7039163	0.5328291
C	4.3721062	3.1111091	-0.1548663
C	-4.0897875	1.9609670	1.3093252
C	-5.6130192	2.5891944	-0.4533245
C	-6.2279791	-1.7049585	-0.5451538
C	-4.3668364	-3.1108357	0.1435021
H	3.3017019	-1.3100584	-1.6772088
C	4.6572828	-2.9161929	-2.1370552
H	5.9512038	-2.4918656	1.4899661
C	6.1532026	-3.5721827	-0.3627945
H	6.6021302	0.7390692	0.8666540
C	7.1026479	2.7761131	0.3632437
H	3.3124463	3.2377952	-0.3536949
C	5.2479822	4.1776968	-0.3236943
H	-3.2779836	1.3375696	1.6743079
C	-4.6505048	2.9269230	2.1430660
H	-5.9816458	2.4665065	-1.4661905
C	-6.1769752	3.5528413	0.3838003
H	-6.5985697	-0.7394101	-0.8757660
C	-7.0959765	-2.7802109	-0.3847115
H	-3.3077886	-3.2356518	0.3466872
C	-5.2406871	-4.1804729	0.3032649
H	4.2820898	-3.0347296	-3.1497470
C	5.6884944	-3.7335418	-1.6690093
H	6.9545061	-4.2029414	0.0121403
H	8.1622466	2.6497882	0.5643742
C	6.6133031	4.0134786	-0.0655203
H	4.8693983	5.1398018	-0.6557801
H	-4.2648700	3.0558662	3.1505481
C	-5.6987380	3.7271777	1.6835769
H	-6.9916822	4.1703516	0.0157732

H	-8.1550273	-2.6555763	-0.5897447
C	-6.6052864	-4.0184671	0.0399263
H	-4.8611196	-5.1432414	0.6322850
H	6.1226059	-4.4910075	-2.3153422
H	7.2936832	4.8496063	-0.1977427
H	-6.1357548	4.4816468	2.3314550
H	-7.2840690	-4.8569918	0.1649816
Cl	4.1046950	-1.0369989	2.6775675
Cl	-4.1025842	1.0514846	-2.6688078

5Cl_2 : adduct of $\mathbf{5}^{2+}$ and two chloride anions
62
Energy = -2307.533390953

H	-1.5086432	-1.9588258	0.2168853
C	-0.8414367	-1.1012640	0.2211522
C	-1.3800206	0.1820974	0.2254539
C	0.5454114	-1.3042206	0.2211894
H	-2.4565590	0.3132786	0.2407470
C	-0.5452493	1.3042096	0.2212844
C	1.3801795	-0.1821106	0.2258991
C	1.0507192	-2.7118100	0.1577933
C	-1.0505793	2.7117810	0.1577921
C	0.8415934	1.1012573	0.2217397
H	2.4567129	-0.3132933	0.2414666
C	0.2177972	-3.9098007	0.3011306
C	0.7115524	-3.6666573	-0.9062395
C	-0.7113943	3.6665640	-0.9062872
C	-0.2177623	3.9098358	0.3011115
H	1.5087994	1.9588223	0.2180064
C	-0.5537486	-4.6650448	1.2460462
C	0.8937960	-3.9268516	-2.3042559
C	-0.8936383	3.9266464	-2.3043207
C	0.5535869	4.6652776	1.2460340
C	-0.6398319	-4.2198938	2.5788760
C	-1.2287194	-5.8415780	0.8670453
C	0.3114913	-5.0498380	-2.9235030
C	1.6673775	-3.0380381	-3.0745957
C	-1.6670230	3.0376224	-3.0746188
C	-0.3115203	5.0496970	-2.9236181
C	1.2285806	5.8417762	0.8669524
C	0.6394844	4.2203565	2.5789520
H	-0.1157239	-3.3141328	2.8686581
C	-1.3860204	-4.9356182	3.5099943
H	-1.1641831	-6.1912260	-0.1587262
C	-1.9744484	-6.5509278	1.8025252
H	-0.2846739	-5.7396025	-2.3340898
C	0.4998503	-5.2728594	-4.2832876
H	2.1156976	-2.1741777	-2.5933575
C	1.8526190	-3.2681316	-4.4341846
H	-2.1153031	2.1737862	-2.5932996
C	-1.8521882	3.2675231	-4.4342463
H	0.2842338	5.7397646	-2.3341609
C	-0.4997852	5.2725105	-4.2834516
H	1.1641926	6.1912776	-0.1588883
C	1.9742488	6.5512408	1.8023935
H	0.1152837	3.3146807	2.8688315
C	1.3855819	4.9362141	3.5100423
H	-1.4476397	-4.5865825	4.5364974
C	-2.0553647	-6.1008066	3.1246426
H	-2.4934385	-7.4570680	1.5040765
H	0.0482587	-6.1402772	-4.7556758
C	1.2698654	-4.3841754	-5.0412675
H	2.4509350	-2.5789712	-5.0227668
H	-2.4502698	2.5781505	-5.0228132
C	-1.2696287	4.3836342	-5.0413864
H	-0.0482124	6.1398904	-4.7559295
H	2.4934569	7.4572106	1.5038085
C	2.0549365	6.1013676	3.1246068
H	1.4471806	4.5872687	4.5365774
H	-2.6381152	-6.6581540	3.8522042
H	1.4153338	-4.5626924	-6.1026977
H	-1.4151439	4.5620843	-6.1028223
H	2.6374717	6.6589083	3.8521922
Cl	2.8086079	-2.8438372	0.8518049
Cl	-2.8085714	2.8437329	0.8516274

5Cl^+ : adduct of $\mathbf{5}^{2+}$ and one chloride
61
Energy = -1847.119400370

H	-1.1249477	-1.8151734	-0.0822728
C	-0.7665851	-0.8363477	-0.3831669
C	0.2702948	-0.2453869	0.3132298
C	-1.3632533	-0.1841624	-1.4819414
H	0.7112785	-0.7608962	1.1586760
C	0.7415040	1.0320728	-0.0591570
C	-0.8902102	1.0829220	-1.8557585
C	-2.4782654	-0.8894606	-2.1780625
C	1.8059227	1.6487699	0.6576443
C	0.1411152	1.6861185	-1.1527468
H	-1.3368204	1.5929816	-2.7003595
C	-2.5975463	-2.3607662	-2.2276414
C	-3.4697528	-1.7233285	-1.4667082
C	2.6147566	2.7508866	0.8979370
C	2.7949920	1.5888866	1.6295626
H	0.4974541	2.6624708	-1.4607241
C	-1.9897360	-3.5198651	-2.8123308
C	-4.5725450	-1.6265365	-0.5563456
C	2.9870081	4.0981651	0.6035878
C	3.4883250	0.8600389	2.6438467
C	-0.8767102	-3.3655922	-3.6598653
C	-2.4866460	-4.8111453	-2.5485913
C	-5.2609955	-2.7771479	-0.1249812
C	-4.9720411	-0.3623160	-0.0839198
C	2.2050535	4.8725431	-0.2776780
C	4.1380886	4.6602389	1.1926923
C	4.4272787	1.5123405	3.4688910
C	3.2366874	-0.5152914	2.8250149
H	-0.5005104	-2.3680705	-3.8663590
C	-0.2724565	-4.4816189	-4.2299888
H	-3.3468133	-4.9344047	-1.8978961

C	-1.8759541	-5.9215504	-3.1208882
H	-4.9586966	-3.7538271	-0.4898840
C	-6.3237108	-2.6592177	0.7639552
H	-4.4431892	0.5232116	-0.4236335
C	-6.0376459	-0.2526857	0.8038311
H	1.3127459	4.4474303	-0.7227193
C	2.5667550	6.1836588	-0.5566513
H	4.7490131	4.0632310	1.8601971
C	4.4988619	5.9685027	0.8998094
H	4.6131985	2.5726200	3.3410271
C	5.0945977	0.8013229	4.4571853
H	2.5248111	-1.0226046	2.1839767
C	3.9166288	-1.2214419	3.8082417
H	0.5847509	-4.3569212	-4.8846920
C	-0.7693002	-5.7602423	-3.9614514
H	-2.2620614	-6.9153352	-2.9149945
H	-6.8516369	-3.5486892	1.0944250
C	-6.7142417	-1.3991984	1.2299240
H	-6.3430592	0.7251988	1.1635948
H	1.9602733	6.7810530	-1.2294488
C	3.7132801	6.7307462	0.0287715
H	5.3887185	6.3979820	1.3481916
H	5.8117145	1.3058291	5.0963991
C	4.8423689	-0.5642711	4.6254011
H	3.7276632	-2.2815299	3.9419866
H	-0.2970958	-6.6303752	-4.4077517
H	-7.5462489	-1.3121308	1.9223628
H	3.9957608	7.7549780	-0.1946797
H	5.3692331	-1.1183881	5.3962027
Cl	-3.0977950	0.0418577	-3.6698848

5^{+}**r** : radical cation

60

Energy = -1386.854435686

H	0.3397466	-2.4334351	-0.3778388
C	0.1954488	-1.3707507	-0.2186816
C	1.2347903	-0.6124852	0.2540445
C	-1.0809464	-0.7885424	-0.4921220
H	2.1877685	-1.0850440	0.4638844
C	1.0805486	0.7885191	0.4911840
C	-1.2349811	0.6125661	-0.2552725
C	-2.1420651	-1.5628021	-0.9751359
C	2.1417180	1.5627756	0.9739819
C	-0.1959038	1.3707337	0.2181977
H	-2.1876747	1.0853438	-0.4657067
C	-2.6648607	-2.7922713	-1.4175675
C	-3.4826528	-1.6931531	-1.3831152
C	2.6638333	2.7915055	1.4191206
C	3.4831387	1.6938115	1.3788327
H	-0.3402875	2.4333512	0.3780220
C	-2.4713880	-4.1831844	-1.6937861
C	-4.7653398	-1.0972296	-1.6021488
C	2.4694144	4.1811738	1.7007972
C	4.7671621	1.0992401	1.5935928
C	-1.1862153	-4.7549381	-1.5962017
C	-3.5607543	-4.9991310	-2.0641426
C	-5.8045407	-1.8341255	-2.2076711
C	-5.0042688	0.2372644	-1.2147191
C	1.1814521	4.7491470	1.6198197
C	3.5608141	4.9992105	2.0603413
C	5.8029013	1.8327999	2.2089631
C	5.0104722	-0.2303301	1.1923368
H	-0.3414170	-4.1340993	-1.3200911
C	-0.9978073	-6.1048313	-1.8666661
H	-4.5550098	-4.5721704	-2.1306241
C	-3.3663453	-6.3489476	-2.3265313
H	-5.6277181	-2.8568814	-2.5206231
C	-7.0458917	-1.2486171	-2.4193158
H	-4.2143378	0.8088375	-0.7406976
C	-6.2507569	0.8147132	-1.4236160
H	0.3354111	4.1262214	1.3522085
C	0.9922095	6.0976320	1.8967514
H	4.5571463	4.5749772	2.1125648
C	3.3654891	6.3477531	2.3286067
H	5.6216631	2.8511206	2.5337747
C	7.0455552	1.2486090	2.4166654
H	4.2228281	-0.7989306	0.7109172
C	6.2584707	-0.8061246	1.3968503
H	-0.0046964	-6.5368265	-1.7936413
C	-2.0857376	-6.9041537	-2.2305321
H	-4.2102521	-6.9715844	-2.6063628
H	-7.8394840	-1.8206569	-2.8895829
C	-7.2726183	0.0748798	-2.0263831
H	-6.4282742	1.8413311	-1.1190453
H	-0.0030547	6.5267735	1.8374993
C	2.0821001	6.8992468	2.2495844
H	4.2107632	6.9723221	2.5998863
H	7.8365809	1.8176680	2.8948179
C	7.2769010	-0.0698624	2.0097329
H	6.4399342	-1.8286122	1.0809126
H	-1.9365684	-7.9592731	-2.4389268
H	-8.2451826	0.5288688	-2.1905728
H	1.9323167	7.9533879	2.4624497
H	8.2504534	-0.5227889	2.1709814

5^{2+} : dication

60

Energy = -1386.681639953

H	0.1871116	-2.4782417	-0.0070609
C	0.1131585	-1.3973834	-0.0137936
C	1.1628840	-0.6312622	0.4627647
C	-1.0592742	-0.7728406	-0.4812807
H	2.0555885	-1.1144213	0.8414159
C	1.0591384	0.7730594	0.4805288
C	-1.1630703	0.6314663	-0.4634600
C	-2.1477651	-1.5670337	-0.9765178
C	2.1476451	1.5671877	0.9757912
C	-0.1132401	1.3975912	0.0128687
H	-2.0557564	1.1146769	-0.8419908
C	-2.6369970	-2.7864788	-1.4077384

C	-3.4694137	-1.6687737	-1.3705991
C	2.6371276	2.7867122	1.4065062
C	3.4690111	1.6685741	1.3708911
H	-0.1868693	2.4785156	0.0054360
C	-2.4327355	-4.1666898	-1.6927647
C	-4.7457993	-1.0710111	-1.5744060
C	2.4335271	4.1672947	1.6902083
C	4.7448804	1.0703644	1.5766406
C	-1.1352132	-4.7177230	-1.6229032
C	-3.5245451	-4.9867471	-2.0479812
C	-5.7816216	-1.8038578	-2.1914134
C	-4.9787715	0.2568701	-1.1566368
C	1.1361404	4.7186860	1.6207501
C	3.5259547	4.9873230	2.0435971
C	5.7794959	1.8024263	2.1965941
C	4.9784320	-0.2571609	1.1580802
H	-0.2923992	-4.0858113	-1.3663122
C	-0.9382425	-6.0610048	-1.9074721
H	-4.5232944	-4.5679933	-2.0915541
C	-3.3192622	-6.3317684	-2.3203239
H	-5.6014694	-2.8199485	-2.5227851
C	-7.0217837	-1.2143323	-2.3908302
H	-4.1894094	0.8164443	-0.6674274
C	-6.2252244	0.8339530	-1.3502204
H	0.2928799	4.0867936	1.3655326
C	0.9398688	6.0623123	1.9042031
H	4.5246610	4.5683563	2.0862837
C	3.3213568	6.3327048	2.3146819
H	5.5986391	2.8180257	2.5291021
C	7.0191305	1.2124711	2.3980226
H	4.1899759	-0.8161404	0.6666984
C	6.2244487	-0.8345782	1.3535239
H	0.0595135	-6.4845375	-1.8616759
C	-2.0286824	-6.8676959	-2.2525578
H	-4.1588589	-6.9648966	-2.5869734
H	-7.8169667	-1.7744567	-2.8712855
C	-7.2443132	0.1009812	-1.9691315
H	-6.4083915	1.8518861	-1.0227226
H	-0.0577672	6.4861763	1.8588413
C	2.0308754	6.8689591	2.2475999
H	4.1613874	6.9659035	2.5797913
H	7.8134365	1.7719376	2.8806878
C	7.2423256	-0.1024345	1.9754041
H	6.4082435	-1.8521253	1.0251732
H	-1.8712912	-7.9195296	-2.4704559
H	-8.2172380	0.5574608	-2.1228647
H	1.8740035	7.9210289	2.4647351
H	8.2148253	-0.5592636	2.1307859

600 : SET reduction of **6**$^{+}$**r**

60

Energy = -1784.132097284

F	0.3278354	-2.7112751	-0.2194359
C	0.1647055	-1.3615606	-0.1423819
C	1.1922563	-0.6124774	0.3239176
C	-1.1248582	-0.8203702	-0.5108855
F	2.3406972	-1.2440140	0.6932853
C	1.1251558	0.8200898	0.5107790
C	-1.1919247	0.6121982	-0.3240358
C	-2.1608131	-1.5762716	-0.9823366
C	2.1610764	1.5760588	0.9822134
C	-0.1644323	1.3612864	0.1423776
F	-2.3403540	1.2437916	-0.6934724
C	-2.7147295	-2.8173064	-1.4280211
C	-3.5179595	-1.7300693	-1.4067075
C	2.7147872	2.8171509	1.4279410
C	3.5182329	1.7300698	1.4065084
F	-0.3276149	2.7109442	0.2197265
C	-2.5777367	-4.2199266	-1.7065152
C	-4.8194987	-1.1773618	-1.6599528
C	2.5774531	4.2196930	1.7066818
C	4.8198707	1.1775806	1.6597010
C	-1.3085040	-4.8165332	-1.8412648
C	-3.7297201	-5.0210691	-1.8593093
C	-5.7438662	-1.8923433	-2.4515600
C	-5.2000762	0.0686981	-1.1237452
C	1.3080711	4.8158730	1.8418794
C	3.7292395	5.0211555	1.8593144
C	5.7442026	1.8927766	2.4511427
C	5.2005863	-0.0684711	1.1235656
H	-0.4208672	-4.2062701	-1.7303313
C	-1.1994238	-6.1734558	-2.1314478
H	-4.7113144	-4.5751133	-1.7364135
C	-3.6117687	-6.3777709	-2.1344230
H	-5.4527996	-2.8431707	-2.8860210
C	-7.0075774	-1.3716761	-2.7007519
H	-4.4975177	0.6195904	-0.5109958
C	-6.4731654	0.5763683	-1.3663196
H	0.4205922	4.2053613	1.7310625
C	1.1986552	6.1727109	2.1323058
H	4.7109507	4.5754719	1.7363071
C	3.6109359	6.3778120	2.1345392
H	5.4530496	2.8436171	2.8855062
C	7.0080207	1.3723448	2.7002369
H	4.4980489	-0.6195387	0.5109416
C	6.4737952	-0.5759040	1.3660347
H	-0.2164661	-6.6218138	-2.2426066
C	-2.3462375	-6.9586756	-2.2759687
H	-4.5050133	-6.9866191	-2.2388429
H	-7.7066736	-1.9257420	-3.3202091
C	-7.3788755	-0.1370861	-2.1558166
H	-6.7600145	1.5335629	-0.9407436
H	0.2155789	6.6206638	2.2440127
C	2.3452566	6.9583085	2.2764585
H	4.5040291	6.9869073	2.2388209
H	7.7070912	1.9266039	3.3195460
C	7.3794711	0.1377700	2.1553731
H	6.7607301	-1.5330732	0.9404586
H	-2.2565130	-8.0183282	-2.4964545
H	-8.3689993	0.2657764	-2.3478451

H	2.2552538	8.0179555	2.4968535
H	8.3696861	-0.2649043	2.3473238

6Cl_2a : higher **6**Cl_2

62

Energy = -2704.663179227

F	1.4316286	-2.1440693	0.8795521
C	0.7400582	-1.0769149	0.4438842
C	-0.6260956	-1.1983170	0.2677715
C	1.4166327	0.1302669	0.1783310
F	-1.2075566	-2.3815148	0.5422892
C	-1.4192868	-0.1293838	-0.1863766
C	0.6234274	1.1992040	-0.2758523
C	2.8253001	0.2388658	0.3679806
C	-2.8282296	-0.2371876	-0.3742796
C	-0.7427083	1.0778045	-0.4519737
F	1.2048201	2.3827620	-0.5491202
C	4.0109845	-0.5279074	0.7817598
C	3.9900690	0.8781563	0.3463603
C	-4.0146874	0.5323857	-0.7806841
C	-3.9933073	-0.8757960	-0.3521218
F	-1.4343175	2.1451600	-0.8871564
C	4.5996110	-1.6490240	-0.0204952
C	4.8641764	1.9931159	0.1326114
C	-4.5993182	1.6500943	0.0292265
C	-4.8671772	-1.9915267	-0.1416651
C	4.9415231	-1.3907326	-1.3565615
C	4.7790377	-2.9397105	0.4868506
C	6.2413392	1.8169257	0.3751431
C	4.3937176	3.2456017	-0.3082136
C	-4.9331333	1.3864201	1.3663013
C	-4.7821540	2.9427425	-0.4718052
C	-6.2457160	-1.8121837	-0.3737041
C	-4.3948375	-3.2481317	0.2852582
H	4.8049483	-0.3922650	-1.7630649
C	5.4532289	-2.4025894	-2.1664158
H	4.5222746	-3.1491140	1.5194024
C	5.2874930	-3.9532752	-0.3266920
H	6.5979940	0.8504317	0.7177877
C	7.1275658	2.8702265	0.1791380
H	3.3353780	3.3862369	-0.4934550
C	5.2869714	4.2929616	-0.5028204
H	-4.7936947	0.3863745	1.7679791
C	-5.4407251	2.3947052	2.1831663
H	-4.5316865	3.1563694	-1.5050289
C	-5.2862910	3.9528063	0.3487784
H	-6.6038261	-0.8425590	-0.7058184
C	-7.1315251	-2.8663727	-0.1806600
H	-3.3351888	-3.3912249	0.4609348
C	-5.2876680	-4.2963727	0.4769546
H	5.7186831	-2.1827141	-3.1966781
C	5.6280206	-3.6901753	-1.6542414
H	5.4185333	-4.9514053	0.0819358
H	8.1872752	2.7281268	0.3681420
C	6.6527904	4.1093245	-0.2608372
H	4.9209777	5.2571112	-0.8429159
H	-5.7000377	2.1705820	3.2140860
C	-5.6187610	3.6843327	1.6772748
H	-5.4200190	4.9525315	-0.0550524
H	-8.1923526	-2.7218298	-0.3613817
C	-6.6549334	-4.1094929	0.2457941
H	-4.9202907	-5.2637601	0.8061971
H	6.0281225	-4.4796670	-2.2839541
H	7.3450905	4.9319459	-0.4141570
H	-6.0154666	4.4711291	2.3124787
H	-7.3469117	-4.9328496	0.3966143
Cl	4.2066131	-0.7934440	2.6204789
Cl	-4.2163829	0.8068093	-2.6172798

6Cl_2 : adduct of $\mathbf{6}^{2+}$ and two chloride anions

62

Energy = -2704.663348752

F	-2.0525067	-1.7857487	0.7833566
C	-1.0127843	-0.9250031	0.7845949
C	-1.2996561	0.4347286	0.7794479
C	0.2981149	-1.4084905	0.7806511
F	-2.5988388	0.8023922	0.7803237
C	-0.2980128	1.4088185	0.7809690
C	1.2997597	-0.4344026	0.7783331
C	0.6128276	-2.8683031	0.7373064
C	-0.6127337	2.8686265	0.7376844
C	1.0128815	0.9253208	0.7837615
F	2.5989408	-0.8020715	0.7781389
C	-0.2025153	-3.9332696	0.1580799
C	0.9315679	-3.6375850	-0.4700464
C	-0.9316591	3.6377795	-0.4697096
C	0.2024978	3.9335725	0.1582255
F	2.0526130	1.7860928	0.7814759
C	-1.3512463	-4.7683337	0.3702537
C	1.9064829	-3.8676351	-1.4982501
C	-1.9065719	3.8674584	-1.4979847
C	1.3511918	4.7687019	0.3703726
C	-2.0533697	-4.6974659	1.5880180
C	-1.7689553	-5.6848259	-0.6136366
C	1.6429646	-4.7815322	-2.5380169
C	3.1397878	-3.1900426	-1.4752058
C	-3.1394601	3.1890844	-1.4753222
C	-1.6433246	4.7816475	-2.5375564
C	1.7688717	5.6853414	-0.6133978
C	2.0533185	4.6977242	1.5881292
H	-1.7278945	-3.9957692	2.3486331
C	-3.1452296	-5.5289725	1.8152767
H	-1.2377523	-5.7396737	-1.5583619
C	-2.8684005	-6.5051299	-0.3840916
H	0.6944300	-5.3078612	-2.5634043
C	2.5902873	-5.0053716	-3.5306204
H	3.3480257	-2.4944191	-0.6704116
C	4.0856632	-3.4241863	-2.4688765
H	-3.3474440	2.4932084	-0.6706760
C	-4.0852082	3.4227597	-2.4692223

H	-0.6950912	5.3085302	-2.5626047
C	-2.5905224	5.0050102	-3.5303863
H	1.2377569	5.7402323	-1.5581750
C	2.8682039	6.5057505	-0.3836967
H	1.7279131	3.9958611	2.3486190
C	3.1450597	5.5293369	1.8155565
H	-3.6782896	-5.4728363	2.7597162
C	-3.5575579	-6.4313313	0.8305317
H	-3.1888188	-7.2045067	-1.1505667
H	2.3776051	-5.7089486	-4.3299926
C	3.8138316	-4.3283136	-3.4990215
H	5.0366349	-2.9005905	-2.4415722
H	-5.0358540	2.8985528	-2.4422613
C	-3.8136599	4.3271985	-3.4991751
H	-2.3780828	5.7088254	-4.3296136
H	3.1885881	7.2052418	-1.1500795
C	3.5572860	6.4319137	0.8309685
H	3.6780926	5.4731273	2.7600060
H	-4.4135342	-7.0757178	1.0084238
H	4.5525295	-4.5064145	-4.2749648
H	-4.5522795	4.5049652	-4.2752701
H	4.4131292	7.0764356	1.0090121
Cl	1.5477423	-3.3109795	2.3357215
Cl	-1.5473456	3.3114929	2.3361334

6Cla^{+} : higher **6**Cl^{+}
61
Energy = -2244.240430386

F	0.5896940	-2.1039803	-1.6569602
C	0.3080326	-0.9661354	-1.0078176
C	1.3357566	-0.2831582	-0.3857331
C	-1.0203783	-0.4924946	-0.9753459
F	2.5827124	-0.7695809	-0.4691728
C	1.1108040	0.9289587	0.2974738
C	-1.2436470	0.7163437	-0.2871540
C	-2.0612292	-1.1971189	-1.6415083
C	2.1701146	1.6342345	0.9322132
C	-0.2153090	1.4078756	0.3216564
F	-2.4862375	1.2196676	-0.2246441
C	-2.3236583	-2.3000046	-2.5796829
C	-3.3331912	-1.4032059	-1.9726875
C	2.6842073	2.8102283	1.4541748
C	3.4420081	1.6457682	1.4818418
F	-0.4937989	2.5417384	0.9817059
C	-2.2076451	-3.7498323	-2.2197916
C	-4.7448661	-1.1965628	-1.9166100
C	2.5621626	4.2009914	1.7442468
C	4.6484275	0.9764608	1.8419018
C	-2.2537220	-4.7759119	-3.1689356
C	-2.0943896	-4.0836129	-0.8617687
C	-5.5675811	-1.9759708	-2.7563353
C	-5.3304959	-0.2556914	-1.0447163
C	1.5193503	4.9622779	1.1763688
C	3.5019517	4.8194151	2.5959896
C	5.7734849	1.7328639	2.2334793
C	4.7202070	-0.4321060	1.8214158
H	-2.3339888	-4.5301591	-4.2221877
C	-2.1878710	-6.1106937	-2.7670218
H	-2.0630930	-3.2959252	-0.1138638
C	-2.0257121	-5.4165425	-0.4626707
H	-5.1093029	-2.6997429	-3.4230901
C	-6.9468447	-1.8100256	-2.7298903
H	-4.7004950	0.3333302	-0.3885548
C	-6.7106249	-0.1007985	-1.0220957
H	0.8066333	4.4891137	0.5119288
C	1.4272624	6.3188624	1.4561051
H	4.2930025	4.2290364	3.0447541
C	3.3899295	6.1724740	2.8825013
H	5.7216066	2.8159483	2.2327162
C	6.9512316	1.0889117	2.5850694
H	3.8517334	-1.0121884	1.5340779
C	5.8983190	-1.0662320	2.1914446
H	-2.2238859	-6.8964921	-3.5161702
C	-2.0729927	-6.4369078	-1.4150273
H	-1.9326762	-5.6566846	0.5925974
H	-7.5774954	-2.4087968	-3.3794909
C	-7.5194769	-0.8733029	-1.8638683
H	-7.1623832	0.6205061	-0.3481153
H	0.6330197	6.9098451	1.0120505
C	2.3566037	6.9223247	2.3101815
H	4.1045834	6.6468082	3.5469423
H	7.8208399	1.6695306	2.8746428
C	7.0126607	-0.3087986	2.5680339
H	5.9535133	-2.1498312	2.1870831
H	-2.0180869	-7.4765471	-1.1056119
H	-8.5976881	-0.7460792	-1.8417008
H	2.2762421	7.9825464	2.5297786
H	7.9331883	-0.8101008	2.8510054
Cl	-1.9168525	-1.9547072	-4.3517656

6Cl^{+} : adduct of **6**$^{2+}$ and one chloride
61
Energy = -2244.240751943

F	0.1109582	-2.6404134	-0.6325899
C	0.1042117	-1.3007527	-0.7232003
C	1.0568637	-0.6000271	0.0013650
C	-0.8447722	-0.6514364	-1.5216692
F	1.9220692	-1.2831107	0.7652176
C	1.1100177	0.8039237	-0.0211205
C	-0.7875232	0.7497161	-1.5459573
C	-1.8948111	-1.4029072	-2.2755617
C	2.0829876	1.5291458	0.7269241
C	0.1527320	1.4582826	-0.8182532
F	-1.6558731	1.4468688	-2.2968643
C	-2.4842769	-2.6890931	-1.9093640
C	-3.2673633	-1.6194038	-1.8003458
C	2.4964673	2.7036356	1.3305781
C	3.3037795	1.5716306	1.3771230
F	0.1703866	2.7971647	-0.9057990
C	-2.2787520	-4.1094713	-1.9318247

C	-4.5334310	-0.9977344	-1.5359989
C	2.2742227	4.0681441	1.6780807
C	4.5162518	0.9439111	1.7867810
C	-1.1234575	-4.6412965	-2.5350422
C	-3.2382740	-4.9840575	-1.3865285
C	-5.5755554	-1.7371184	-0.9415936
C	-4.7536495	0.3493726	-1.8790220
C	0.9989486	4.6484635	1.5158375
C	3.3364782	4.8367586	2.1993144
C	5.3520309	1.5865417	2.7245556
C	4.8893341	-0.3067190	1.2515069
H	-0.3887475	-3.9681962	-2.9642880
C	-0.9360925	-6.0182974	-2.5922897
H	-4.1296001	-4.5812041	-0.9167630
C	-3.0389759	-6.3592407	-1.4382964
H	-5.4121616	-2.7746474	-0.6693565
C	-6.8048437	-1.1373796	-0.6935432
H	-3.9586698	0.9159379	-2.3497033
C	-5.9898077	0.9397587	-1.6352074
H	0.1817750	4.0528177	1.1275299
C	0.7958352	5.9740324	1.8738125
H	4.3198343	4.3932968	2.3086908
C	3.1263903	6.1658613	2.5380592
H	5.0554197	2.5401710	3.1468510
C	6.5333522	0.9799996	3.1268839
H	4.2524231	-0.7927217	0.5223858
C	6.0820831	-0.8957721	1.6478209
H	-0.0461202	-6.4224195	-3.0651635
C	-1.8896344	-6.8795073	-2.0417171
H	-3.7797286	-7.0279168	-1.0104143
H	-7.6015453	-1.7125911	-0.2317154
C	-7.0159923	0.2010601	-1.0403349
H	-6.1547144	1.9774120	-1.9092250
H	-0.1863726	6.4207950	1.7600716
C	1.8570800	6.7326477	2.3795165
H	3.9449349	6.7619162	2.9276958
H	7.1716165	1.4669370	3.8567216
C	6.9001856	-0.2571737	2.5860724
H	6.3779658	-1.8523301	1.2299348
H	-1.7388551	-7.9541498	-2.0837097
H	-7.9785476	0.6655625	-0.8481386
H	1.6939127	7.7707041	2.6525856
H	7.8291851	-0.7254201	2.8966938
Cl	-1.6079212	-1.0798219	-4.1146174

6^{+}r : radical cation

60

Energy = -1783.984208533

F	0.2188289	-2.7199441	0.0198915
C	0.1154782	-1.3764259	-0.0284769
C	1.1531899	-0.6192322	0.4436216
C	-1.0975524	-0.8009239	-0.5094979
F	2.2397254	-1.2452622	0.9391904
C	1.1033801	0.8052037	0.4923772
C	-1.1467459	0.6236409	-0.4619810
C	-2.1574488	-1.5740584	-0.9892243
C	2.1617309	1.5778276	0.9763010
C	-0.1091378	1.3808270	0.0103320
F	-2.2331165	1.2497958	-0.9577655
C	-2.6812969	-2.8046880	-1.4190057
C	-3.4950625	-1.7017381	-1.3995501
C	2.6830191	2.8066722	1.4142094
C	3.4980407	1.7047134	1.3906734
F	-0.2119953	2.7243903	-0.0385580
C	-2.5275201	-4.2011547	-1.6955214
C	-4.7895540	-1.1379650	-1.6373240
C	2.5261203	4.2007847	1.7002729
C	4.7920509	1.1401523	1.6291372
C	-1.2483312	-4.7788275	-1.8201832
C	-3.6739583	-5.0071356	-1.8582393
C	-5.7280442	-1.8549284	-2.4091365
C	-5.1438603	0.1159755	-1.1009949
C	1.2454576	4.7754624	1.8238017
C	3.6706198	5.0070303	1.8749656
C	5.7264793	1.8508235	2.4115541
C	5.1495706	-0.1086215	1.0830143
H	-0.3669986	-4.1593879	-1.7084076
C	-1.1244637	-6.1331143	-2.1078005
H	-4.6597809	-4.5687227	-1.7455346
C	-3.5394400	-6.3626967	-2.1276445
H	-5.4522306	-2.8126132	-2.8375937
C	-6.9875151	-1.3206979	-2.6466797
H	-4.4296154	0.6622763	-0.4974439
C	-6.4131951	0.6341357	-1.3299136
H	0.3655833	4.1557898	1.7021372
C	1.1182165	6.1269342	2.1229384
H	4.6575969	4.5709911	1.7630387
C	3.5327831	6.3599504	2.1556892
H	5.4478338	2.8041884	2.8477927
C	6.9851829	1.3151819	2.6500698
H	4.4382186	-0.6500878	0.4716712
C	6.4183446	-0.6278336	1.3126367
H	-0.1381914	-6.5736452	-2.2144669
C	-2.2656856	-6.9268217	-2.2569433
H	-4.4236363	-6.9821633	-2.2394828
H	-7.7023451	-1.8694381	-3.2515929
C	-7.3335842	-0.0782678	-2.1044648
H	-6.6876547	1.5951999	-0.9065379
H	0.1308060	6.5650025	2.2291954
C	2.2575611	6.9209274	2.2844331
H	4.4154782	6.9797745	2.2769967
H	7.6969048	1.8588436	3.2631804
C	7.3345781	0.0779958	2.0980731
H	6.6954664	-1.5847325	0.8816384
H	-2.1634712	-7.9856379	-2.4748377
H	-8.3216442	0.3339002	-2.2857333
H	2.1527463	7.9775396	2.5115921
H	8.3220839	-0.3351652	2.2801110

6^{2+} : dication

60
Energy = -1783.800550185

F	-0.0060743	-2.6890132	0.4317100
C	-0.0018149	-1.3735492	0.1958440
C	1.0489260	-0.6081404	0.6745970
C	-1.0775033	-0.7853466	-0.4925646
F	2.0290412	-1.2073204	1.3577152
C	1.0785510	0.7854103	0.4901767
C	-1.0477602	0.6081708	-0.6772030
C	-2.1638103	-1.5772877	-0.9871785
C	2.1644949	1.5774136	0.9854857
C	0.0029363	1.3735903	-0.1983572
F	-2.0276508	1.2072734	-1.3606470
C	-2.6494607	-2.7968596	-1.4169190
C	-3.4846677	-1.6761265	-1.3791259
C	2.6496932	2.7969390	1.4158655
C	3.4850086	1.6762438	1.3785664
F	0.0071180	2.6890999	-0.4340934
C	-2.4559288	-4.1742379	-1.7096430
C	-4.7648540	-1.0922212	-1.5801203
C	2.4558788	4.1742953	1.7085517
C	4.7649582	1.0922834	1.5809316
C	-1.1552495	-4.7237610	-1.7277775
C	-3.5721797	-4.9926185	-1.9899822
C	-5.7661144	-1.8204499	-2.2593973
C	-5.0404108	0.2061215	-1.0981017
C	1.1552281	4.7239572	1.7248378
C	3.5717513	4.9925490	1.9907327
C	5.7655233	1.8204230	2.2613267
C	5.0409786	-0.2060831	1.0992660
H	-0.2990367	-4.0911051	-1.5271893
C	-0.9819246	-6.0673583	-2.0246464
H	-4.5709480	-4.5723391	-1.9603595
C	-3.3874814	-6.3382555	-2.2698466
H	-5.5477306	-2.8107832	-2.6422505
C	-7.0146405	-1.2518997	-2.4618235
H	-4.2757382	0.7574717	-0.5643615
C	-6.2977277	0.7579887	-1.2929001
H	0.2992415	4.0914413	1.5228008
C	0.9815835	6.0675206	2.0216999
H	4.5704976	4.5721647	1.9624929
C	3.3867892	6.3381268	2.2706251
H	5.5467723	2.8108019	2.6438335
C	7.0137387	1.2517643	2.4653212
H	4.2768824	-0.7574126	0.5646821
C	6.2980137	-0.7580550	1.2955465
H	0.0158297	-6.4924337	-2.0501521
C	-2.0947675	-6.8738491	-2.2905538
H	-4.2436072	-6.9723287	-2.4740279
H	-7.7823235	-1.8040315	-2.9933326
C	-7.2811255	0.0333121	-1.9764751
H	-6.5181215	1.7509556	-0.9156510
H	-0.0161698	6.4926809	2.0456458
C	2.0940926	6.8738290	2.2895326
H	4.2426621	6.9721007	2.4761758
H	7.7808175	1.8037804	2.9978335
C	7.2806852	-0.0334605	1.9802455
H	6.5186951	-1.7510936	0.9186731
H	-1.9533357	-7.9261562	-2.5169068
H	-8.2619168	0.4725436	-2.1304091
H	1.9524093	7.9260755	2.5160059
H	8.2612770	-0.4727513	2.1352748

700 : SET reduction of **7**$^{+}$**r**
60
Energy = -3769.755814341

F	0.1965982	-2.7334455	0.0765485
C	0.1238190	-1.3816328	-0.0150181
C	1.1504951	-0.6310006	0.4501940
C	-1.1116334	-0.8124790	-0.5037384
F	2.2280443	-1.2481437	0.9971042
C	1.1116123	0.8128534	0.5036625
C	-1.1504651	0.6313758	-0.4503590
C	-2.1436131	-1.5665024	-0.9710770
C	2.1435995	1.5668380	0.9710368
C	-0.1238613	1.3820099	0.0150140
F	-2.2278500	1.2485484	-0.9975944
C	-2.6996506	-2.8054674	-1.4182812
C	-3.5008135	-1.7247495	-1.3926473
C	2.6997370	2.8057263	1.4183449
C	3.5007964	1.7249446	1.3926343
F	-0.1967715	2.7338301	-0.0762390
C	-2.5797340	-4.2031767	-1.6925316
C	-4.7980347	-1.1864011	-1.6581135
C	2.5799628	4.2034524	1.6925733
C	4.7978956	1.1863113	1.6581497
C	-1.3723105	-4.7842815	-2.1202620
C	-3.6894488	-5.0582091	-1.5559263
C	-5.6085523	-1.7344555	-2.6701045
C	-5.3277291	-0.1071701	-0.9278955
C	1.3726090	4.7847067	2.1202856
C	3.6897440	5.0583701	1.5558243
C	5.6082706	1.7338117	2.6705413
C	5.3275134	0.1072252	0.9276745
F	-0.3000603	-4.0112595	-2.3392454
C	-1.2720024	-6.1426374	-2.3888324
F	-4.8577250	-4.5604648	-1.1176232
C	-3.6037443	-6.4181972	-1.8121578
F	-5.1379097	-2.7452601	-3.4194068
C	-6.8673183	-1.2285248	-2.9568093
F	-4.6361460	0.4092840	0.0969288
C	-6.5891896	0.4060189	-1.1972016
F	0.3002568	4.0118245	2.3392687
C	1.2724510	6.1430924	2.3887494
F	4.8579672	4.5604406	1.1175756
C	3.6041532	6.4184131	1.8118024
F	5.1376543	2.7444750	3.4200575
C	6.8668137	1.2274329	2.9574479
F	4.6359924	-0.4087972	-0.0974108
C	6.5888144	-0.4063021	1.1970693

F	-0.1161935	-6.6686176	-2.8211194
C	-2.3891329	-6.9623188	-2.2313475
F	-4.6701977	-7.2152936	-1.6477548
F	-7.6073868	-1.7517149	-3.9459698
C	-7.3596539	-0.1533152	-2.2161175
F	-7.0819695	1.4199370	-0.4701985
F	0.1167249	6.6692155	2.8210971
C	2.3896180	6.9626797	2.2310249
F	4.6706595	7.2153911	1.6471974
F	7.6067148	1.7500654	3.9470241
C	7.3591101	0.1524156	2.2164515
F	7.0815884	-1.4200099	0.4697612
F	-2.2985018	-8.2710608	-2.4889835
F	-8.5752815	0.3368182	-2.4795065
F	2.2991007	8.2714694	2.4884742
F	8.5745651	-0.3380885	2.4799543

7Cl_2a : higher **7**Cl_2

62

Energy = -4690.283142871

F	1.2058521	-1.2348540	2.1074375
C	0.6272417	-0.6377291	1.0546952
C	-0.7441609	-0.7514057	0.8918992
C	1.4138101	0.1219728	0.1720851
F	-1.4478504	-1.4312893	1.8106364
C	-1.4137933	-0.1234920	-0.1731045
C	0.7442163	0.7497684	-0.8929898
C	2.8361467	0.2088637	0.3187373
C	-2.8362514	-0.2095330	-0.3192654
C	-0.6271816	0.6360873	-1.0558023
F	1.4479291	1.4298179	-1.8116063
C	4.0569147	-0.5548130	0.6654201
C	3.9933633	0.8421491	0.2103185
C	-4.0567321	0.5549633	-0.6653277
C	-3.9938552	-0.8421447	-0.2106948
F	-1.2056832	1.2328670	-2.1087748
C	4.5203735	-1.7114365	-0.1649658
C	4.7678476	2.0331340	0.0687164
C	-4.5194028	1.7114175	0.1656762
C	-4.7691195	-2.0326616	-0.0693834
C	5.3270371	-1.5482474	-1.2953026
C	4.0970813	-3.0174558	0.1124187
C	6.1621877	2.0268414	0.2653298
C	4.1672460	3.2766701	-0.2012997
C	-5.3251702	1.5476608	1.2966742
C	-4.0958454	3.0173610	-0.1115123
C	-6.1634707	-2.0252382	-0.2658925
C	-4.1694520	-3.2767503	0.2001260
F	5.7304123	-0.3197363	-1.6776379
C	5.7280957	-2.6213974	-2.0861494
F	3.2690060	-3.2519746	1.1462225
C	4.4900074	-4.1066044	-0.6571669
F	6.7934615	0.8871658	0.5783521
C	6.9193484	3.1858174	0.1647740
F	2.8365498	3.3532270	-0.3410867
C	4.9093757	4.4433165	-0.3061466
F	-5.7288421	0.3194622	1.6784036
C	-5.7248866	2.6207583	2.0883908
F	-3.2686468	3.2520336	-1.1460421
C	-4.4876664	4.1063058	0.6589024
F	-6.7938870	-0.8849815	-0.5784760
C	-6.9214926	-3.1837017	-0.1658361
F	-2.8388071	-3.3544149	0.3397106
C	-4.9124742	-4.4428626	0.3046377
F	6.5083332	-2.4180943	-3.1599871
C	5.3144171	-3.9088980	-1.7616258
F	4.0674323	-5.3435598	-0.3506829
F	8.2458553	3.1515451	0.3541020
C	6.2920912	4.3960712	-0.1272650
F	4.3108176	5.6137602	-0.5670530
F	-6.5041501	2.4175287	3.1629759
C	-5.3110073	3.9082491	1.7640934
F	-4.0650476	5.3433206	0.3525448
F	-8.2480166	-3.1483183	-0.3549048
C	-6.2951453	-4.3945433	0.1257177
F	-4.3148039	-5.6138478	0.5651895
F	5.6944509	-4.9493493	-2.5141679
F	7.0143314	5.5148135	-0.2237344
F	-5.6897469	4.9484687	2.5176893
F	-7.0182175	-5.5127925	0.2217073
Cl	4.4908532	-0.7972446	2.4377118
Cl	-4.4912800	0.7979536	-2.4374112

7Cl_2 : adduct of $\mathbf{7}^{2+}$ and two chloride anions

62

Energy = -4690.285780809

F	-2.2153562	-1.7166024	0.7128647
C	-1.1717750	-0.8608786	0.6953379
C	-1.4535493	0.5010472	0.6891821
C	0.1360160	-1.3484634	0.6795033
F	-2.7471722	0.8732542	0.6627089
C	-0.4424415	1.4673744	0.6920178
C	1.1475740	-0.3847885	0.6505292
C	0.4481635	-2.8084605	0.7166600
C	-0.7488902	2.9323091	0.6552498
C	0.8668246	0.9762099	0.6498832
F	2.4386589	-0.7627827	0.6249523
C	0.6993086	-3.5864492	1.9476174
C	-0.4025794	-3.8661919	1.2743914
C	-0.7945508	3.6848310	-0.6185752
C	0.1871548	3.9782671	0.2178355
F	1.9136050	1.8264145	0.5906013
C	1.6317685	-3.8980919	2.9933187
C	-1.5804638	-4.6571817	1.0963795
C	-1.4801922	3.8057101	-1.8727766
C	1.2628071	4.8028531	0.6683069
C	2.3592235	-2.9014525	3.6607304
C	1.8631548	-5.2291038	3.3789826
C	-2.0948118	-5.4285324	2.1526411
C	-2.2823931	-4.6845253	-0.1201055

C	-2.8707396	3.6317697	-1.9686260
C	-0.7828266	4.0466950	-3.0692406
C	1.7125378	5.9069861	-0.0777377
C	1.8766580	4.5830348	1.9158675
F	2.1503947	-1.6114772	3.3555724
C	3.2688781	-3.2060442	4.6646064
F	1.2267980	-6.2263238	2.7449169
C	2.7742833	-5.5539601	4.3750016
F	-1.4861496	-5.4007085	3.3489728
C	-3.2406962	-6.1969175	2.0091634
F	-1.8388446	-3.9712892	-1.1647247
C	-3.4272858	-5.4529697	-0.2836250
F	-3.5888443	3.4033668	-0.8591261
C	-3.5386653	3.7184529	-3.1833417
F	0.5549487	4.1519778	-3.0516616
C	-1.4335926	4.1264533	-4.2931884
F	1.1263847	6.1996183	-1.2474284
C	2.7377402	6.7270372	0.3692440
F	1.4632956	3.5796525	2.7024331
C	2.9038891	5.3942326	2.3781218
F	3.9362160	-2.2326850	5.3006012
C	3.4770192	-4.5376421	5.0209470
F	2.9925459	-6.8339155	4.7110237
F	-3.7164272	-6.9158149	3.0361328
C	-3.9068287	-6.2111859	0.7836104
F	-4.0718588	-5.4743925	-1.4590906
F	-4.8703035	3.5710805	-3.2401872
C	-2.8175290	3.9677889	-4.3497183
F	-0.7399803	4.3405968	-5.4208537
F	3.1474653	7.7714880	-0.3648119
C	3.3393062	6.4657833	1.6002119
F	3.4749997	5.1591316	3.5679734
F	4.3530134	-4.8408136	5.9839422
F	-5.0093382	-6.9510038	0.6336867
F	-3.4518564	4.0479682	-5.5237070
F	4.3264812	7.2511305	2.0393872
Cl	1.4264473	-3.2749110	-0.7953507
Cl	-1.8910655	3.4072465	2.0203503

7Cl^+ : adduct of $\mathbf{7}^{2+}$ and one chloride

61

Energy = -4229.846267862

F	-0.2235777	-2.5799456	-0.4499387
C	-0.0687119	-1.2685883	-0.6911860
C	0.8749869	-0.5875513	0.0617902
C	-0.8600862	-0.6221532	-1.6534051
F	1.5759437	-1.2529490	0.9849501
C	1.0633243	0.7982168	-0.0897307
C	-0.6861321	0.7664574	-1.7826968
C	-1.9051131	-1.3549396	-2.4351543
C	2.0162151	1.5097334	0.6843337
C	0.2514529	1.4575327	-1.0325337
F	-1.4379118	1.4685307	-2.6394391
C	-2.4452167	-2.6767103	-2.0780322
C	-3.2320527	-1.6418346	-1.8366364
C	2.4531203	2.7003502	1.2360812
C	3.1788270	1.5390534	1.4351697
F	0.4146494	2.7683667	-1.2394775
C	-2.2060873	-4.0744333	-2.2381886
C	-4.4251814	-1.0422357	-1.3170795
C	2.2907869	4.0944362	1.4432008
C	4.2936808	0.8833835	2.0157130
C	-0.9695208	-4.5521479	-2.7115766
C	-3.2123600	-5.0286194	-2.0000614
C	-5.0903942	-1.5899805	-0.2058156
C	-4.9521748	0.1415627	-1.8599286
C	1.0142088	4.6923437	1.4148371
C	3.4062046	4.9246424	1.6780528
C	4.9227124	1.4153442	3.1610614
C	4.8045561	-0.3155368	1.4766094
F	0.0174942	-3.6899704	-2.9978137
C	-0.7360194	-5.9054961	-2.9090993
F	-4.4266379	-4.6255006	-1.6030221
C	-2.9953854	-6.3849450	-2.1910945
F	-4.5932352	-2.6807424	0.3955937
C	-6.2295891	-1.0023863	0.3270081
F	-4.3573149	0.7054268	-2.9216723
C	-6.0962700	0.7371877	-1.3451435
F	-0.0690350	3.9275265	1.2554621
C	0.8530679	6.0534221	1.6158853
F	4.6345054	4.4001841	1.6573129
C	3.2607938	6.2896296	1.8633714
F	4.4308515	2.5188615	3.7303535
C	6.0039483	0.7808352	3.7492513
F	4.2689797	-0.8191069	0.3627296
C	5.8952982	-0.9520355	2.0460051
F	0.4518526	-6.3343915	-3.3557112
C	-1.7505355	-6.8246518	-2.6426556
F	-3.9705229	-7.2724994	-1.9568168
F	-6.8343009	-1.5364823	1.3965002
C	-6.7378166	0.1619274	-0.2487627
F	-6.5894757	1.8538725	-1.8971190
F	-0.3613888	6.6058643	1.6175577
C	1.9805472	6.8504484	1.8355569
F	4.3250891	7.0718280	2.0518396
F	6.5723233	1.2758472	4.8501360
C	6.4905188	-0.4025486	3.1856280
F	6.3901447	-2.0703873	1.5127861
F	-1.5339258	-8.1273191	-2.8307902
F	-7.8361115	0.7296962	0.2548269
F	1.8335926	8.1559472	2.0204083
F	7.5301451	-1.0121886	3.7397267
Cl	-1.7640725	-1.0000430	-4.2257649

$\mathbf{7}^+\mathbf{r}$: radical cation

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Energy = -3769.591662964

F	0.0813909	-2.7136405	0.2871760
C	0.0663379	-1.3842598	0.0923258
C	1.1032849	-0.6249447	0.5657199

C	-1.0817298	-0.7958003	-0.5147580
F	2.1152616	-1.2247750	1.2149393
C	1.0953199	0.7982344	0.4789942
C	-1.0884285	0.6273049	-0.6037665
C	-2.1389011	-1.5675348	-0.9915091
C	2.1480991	1.5703671	0.9647616
C	-0.0515015	1.3864760	-0.1305314
F	-2.0999897	1.2269025	-1.2537511
C	-2.6670889	-2.7962032	-1.4192806
C	-3.4761133	-1.6976025	-1.3989255
C	2.6699588	2.7975842	1.4045884
C	3.4813451	1.7007446	1.3843748
F	-0.0665030	2.7158897	-0.3247584
C	-2.5119954	-4.1871070	-1.6821762
C	-4.7591663	-1.1268857	-1.6351343
C	2.5093418	4.1856099	1.6790138
C	4.7627324	1.1306277	1.6310453
C	-1.2681688	-4.7363489	-2.0475271
C	-3.6120212	-5.0623226	-1.5922400
C	-5.6246845	-1.6768912	-2.6007440
C	-5.2131774	-0.0070086	-0.9127654
C	1.2608726	4.7288402	2.0375307
C	3.6083379	5.0639426	1.6082022
C	5.6147773	1.6734746	2.6124299
C	5.2273495	0.0174289	0.9052473
F	-0.2094171	-3.9343654	-2.2060156
C	-1.1247318	-6.0903258	-2.3106978
F	-4.8025472	-4.5879894	-1.2041546
C	-3.4812910	-6.4197416	-1.8394850
F	-5.2140178	-2.7152276	-3.3395867
C	-6.8755659	-1.1334251	-2.8473872
F	-4.4520513	0.5095030	0.0584163
C	-6.4668046	0.5403039	-1.1400110
F	0.2022496	3.9233739	2.1778768
C	1.1123939	6.0795508	2.3141481
F	4.8036885	4.5956358	1.2276552
C	3.4727219	6.4183302	1.8691037
F	5.1929215	2.7049869	3.3546042
C	6.8631725	1.1296361	2.8705806
F	4.4788800	-0.4923962	-0.0792910
C	6.4791183	-0.5295834	1.1433653
F	0.0575136	-6.5920188	-2.6832524
C	-2.2334175	-6.9322891	-2.2018070
F	-4.5296572	-7.2410695	-1.7208916
F	-7.6736429	-1.6504519	-3.7873498
C	-7.2960396	-0.0227226	-2.1121735
F	-6.8941459	1.5872589	-0.4263725
F	-0.0743886	6.5750333	2.6805074
C	2.2204698	6.9246056	2.2251906
F	4.5205359	7.2428850	1.7694732
F	7.6479700	1.6393516	3.8255815
C	7.2948425	0.0260628	2.1311069
F	6.9173366	-1.5695352	0.4260823
F	-2.1008558	-8.2333781	-2.4484209
F	-8.4984285	0.5011725	-2.3378648
F	2.0831014	8.2226105	2.4850373
F	8.4951466	-0.4978835	2.3675503

7^{2+} : dication

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Energy = -3769.390409222

F	-0.1304723	-2.6457844	0.6170782
C	-0.0562959	-1.3572414	0.2867355
C	0.9957498	-0.5911754	0.7653914
C	-1.0748230	-0.7745830	-0.4891522
F	1.9142479	-1.1570912	1.5471752
C	1.0674879	0.7854940	0.4860281
C	-1.0030812	0.6020352	-0.7686272
C	-2.1589295	-1.5660608	-0.9828597
C	2.1533560	1.5748796	0.9788935
C	0.0486686	1.3683258	-0.2890281
F	-1.9221387	1.1683273	-1.5493364
C	-2.6446763	-2.7858913	-1.4044444
C	-3.4754070	-1.6671561	-1.3812193
C	2.6450180	2.7925079	1.4002333
C	3.4700453	1.6697316	1.3778428
F	0.1229479	2.6566919	-0.6197685
C	-2.4267359	-4.1574975	-1.6669479
C	-4.7344885	-1.0608007	-1.5928773
C	2.4358388	4.1654718	1.6625546
C	4.7251275	1.0559996	1.5924950
C	-1.1234082	-4.6414678	-1.9168139
C	-3.4927304	-5.0836911	-1.6794594
C	-5.6742675	-1.6129449	-2.4910229
C	-5.0847633	0.1261189	-0.9115716
C	1.1358770	4.6591377	1.9113281
C	3.5087957	5.0836972	1.6760119
C	5.6633556	1.5990441	2.4976994
C	5.0709924	-0.1315042	0.9099826
F	-0.1008280	-3.7832217	-1.9551328
C	-0.8915923	-5.9787593	-2.1851629
F	-4.7260093	-4.6736897	-1.3824752
C	-3.2718187	-6.4275459	-1.9294835
F	-5.3517990	-2.6951012	-3.1995787
C	-6.9042395	-1.0126803	-2.7004794
F	-4.2352514	0.6479430	-0.0230879
C	-6.3172993	0.7261543	-1.0991132
F	0.1069966	3.8084920	1.9494386
C	0.9139426	5.9982991	2.1786606
F	4.7393067	4.6640089	1.3810537
C	3.2978348	6.4292897	1.9251936
F	5.3445568	2.6819307	3.2068828
C	6.8870555	0.9884358	2.7140950
F	4.2233748	-0.6442900	0.0143917
C	6.2975376	-0.7416016	1.1042336
F	0.3370213	-6.4219272	-2.4509383
C	-1.9701285	-6.8705304	-2.1877474
F	-4.2776499	-7.3012501	-1.9108051
F	-7.7746607	-1.5225760	-3.5708465
C	-7.2245300	0.1542046	-1.9983091

F	-6.6523904	1.8283737	-0.4288965
F	-0.3114364	6.4510742	2.4431230
C	1.9992580	6.8820681	2.1816410
F	4.3102893	7.2953260	1.9073577
F	7.7554198	1.4891008	3.5918697
C	7.2028095	-0.1793890	2.0114956
F	6.6286287	-1.8445471	0.4331476
F	-1.7544361	-8.1532086	-2.4346635
F	-8.4019305	0.7283655	-2.1899656
F	1.7927264	8.1665121	2.4273208
F	8.3739511	-0.7638339	2.2104590

8$^+$: adduct of **1**$^+$ and PPh_3

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Energy = -1615.164497839

H	-0.8626927	-0.0100215	-2.2909435
C	-0.4223214	0.2969271	-1.3387721
C	-0.5757300	1.7100113	-0.8203146
C	0.6085700	1.3966796	-1.2926430
C	-1.5020581	2.5667018	-0.1456720
C	1.9912687	1.6492033	-1.5664188
C	-1.1203523	3.8654443	0.2476615
C	-2.7910657	2.1039468	0.1766573
C	2.5686743	2.8990646	-1.2624329
C	2.7980528	0.6352552	-2.1169906
H	-0.1280015	4.2306649	0.0041107
C	-2.0087797	4.6713155	0.9492566
H	-3.0868968	1.1041128	-0.1230142
C	-3.6745947	2.9147857	0.8809147
H	1.9538281	3.6867478	-0.8391898
C	3.9197030	3.1198570	-1.5019911
H	2.3547326	-0.3266173	-2.3525105
C	4.1502517	0.8636872	-2.3517410
C	-3.2864090	4.1993649	1.2696972
H	-1.7066586	5.6695825	1.2512831
H	-4.6660019	2.5474799	1.1284334
H	4.3577738	4.0846077	-1.2645414
C	4.7148715	2.1042546	-2.0448102
H	4.7655241	0.0754094	-2.7751117
H	-3.9762963	4.8322883	1.8197265
H	5.7704048	2.2813376	-2.2278350
P	-0.3091048	-1.0452122	-0.1147028
C	1.0255272	-2.1779269	-0.5255078
C	1.9504382	-2.6065342	0.4352581
C	1.1059844	-2.6499822	-1.8465513
C	2.9648174	-3.4905881	0.0680017
H	1.8818042	-2.2537365	1.4590137
C	2.1217441	-3.5316333	-2.2028167
H	0.3836045	-2.3297929	-2.5923591
C	3.0534909	-3.9480492	-1.2471013
H	3.6842558	-3.8196848	0.8110809
H	2.1871995	-3.8926589	-3.2243058
H	3.8468209	-4.6333988	-1.5292934
C	-0.0030802	-0.2698353	1.4705427
C	1.2265457	0.3724595	1.6952760
C	-1.0312231	-0.1790564	2.4188208
C	1.4201006	1.0966037	2.8677360
H	2.0220041	0.3102929	0.9592289
C	-0.8256878	0.5451073	3.5909708
H	-1.9845571	-0.6650326	2.2383721
C	0.3951774	1.1837132	3.8134200
H	2.3691990	1.5931947	3.0432681
H	-1.6201452	0.6124849	4.3271841
H	0.5505996	1.7502220	4.7264770
C	-1.8411753	-1.9808326	-0.0702398
C	-1.8999611	-3.1355849	0.7275813
C	-2.9585365	-1.5791884	-0.8145593
C	-3.0806456	-3.8687854	0.7924482
H	-1.0292794	-3.4567204	1.2924894
C	-4.1350403	-2.3250614	-0.7494604
H	-2.9126391	-0.7011245	-1.4499204
C	-4.1973829	-3.4631610	0.0553512
H	-3.1288217	-4.7579077	1.4130418
H	-4.9991254	-2.0170643	-1.3294324
H	-5.1154883	-4.0405113	0.1047825

A$^+$: unstable adduct of **2**$^+$ and alkyne

54

Energy = -1232.733434375

C	-1.0511455	-1.7932466	0.0300311
C	-1.6215659	-1.5089389	-1.2204810
C	-1.2675941	-3.0530130	0.6004831
C	-0.2126001	-0.7463723	0.7104993
H	-1.4603284	-0.5347228	-1.6735849
C	-2.3925241	-2.4630763	-1.8792665
H	-0.8254460	-3.2960863	1.5627614
C	-2.0420208	-4.0089149	-0.0603587
C	-0.2949506	0.7056756	0.3375056
C	0.7842752	0.0624257	-0.0613817
C	-2.6067494	-3.7180680	-1.3020348
H	-2.8299451	-2.2255398	-2.8449527
H	-2.1996604	-4.9816533	0.3968617
C	-1.1507598	1.8481802	0.4526626
C	2.0513745	-0.0572225	-0.7163728
H	-3.2081788	-4.4611721	-1.8174149
C	-2.4155018	1.7125579	1.0568768
C	-0.7494397	3.1093525	-0.0321686
C	2.7034518	1.0654015	-1.2645051
C	2.6754114	-1.3180967	-0.7864166
H	-2.7276293	0.7389120	1.4229069
C	-3.2588352	2.8129949	1.1727144
H	0.2250006	3.2209159	-0.4975418
C	-1.5978150	4.2042583	0.0874370
H	2.2280789	2.0400678	-1.2147329
C	3.9545890	0.9255679	-1.8544996
H	2.1655643	-2.1838897	-0.3744887
C	3.9262364	-1.4505915	-1.3785787
C	-2.8527925	4.0600430	0.6892468
H	-4.2334633	2.7003095	1.6379302
H	-1.2834748	5.1734917	-0.2880836

H	4.4547286	1.7948843	-2.2707749
C	4.5700453	-0.3295866	-1.9113194
H	4.4000186	-2.4263491	-1.4298538
H	-3.5120423	4.9181759	0.7798393
H	5.5475764	-0.4327512	-2.3728491
C	0.0654201	-1.0530364	2.1986264
C	1.2740814	-1.2576936	2.5831890
H	-0.7854368	-1.0862983	2.8778836
C	2.6034174	-1.3794516	2.8226517
C	3.2345245	-2.6658061	2.7871479
C	3.4099771	-0.2112221	3.0482929
C	4.5916164	-2.7826705	2.9362552
H	2.6208731	-3.5457389	2.6284042
C	4.7622275	-0.3294032	3.1968297
H	2.9278204	0.7591360	3.0842073
C	5.3696523	-1.6126476	3.1374341
H	5.0601408	-3.7579863	2.9003669
H	5.3960401	0.5354132	3.3591926
O	6.6883956	-1.6217006	3.2816501
C	7.4064774	-2.8894022	3.2410607
H	7.2593988	-3.3656706	2.2689949
H	8.4499784	-2.6180505	3.3816400
H	7.0612614	-3.5340302	4.0521681

Bf_3Cl^- : adduct of $B(C_6F_5)_3$ and chloride
35
Energy = -2669.945762765

B	0.1014441	0.0664021	0.7491166
C	0.5158208	1.5174255	0.1127971
C	-0.2863073	2.2884805	-0.7302213
C	1.7569510	2.0991709	0.4004348
C	0.0726454	3.5477864	-1.2100455
C	2.1567924	3.3498666	-0.0544643
C	1.3022410	4.0897064	-0.8647024
C	-1.4919341	-0.2820985	0.6003756
C	-2.0178479	-1.3538751	-0.1229813
C	-2.4636849	0.5094079	1.2253580
C	-3.3768768	-1.6598481	-0.1853430
C	-3.8272229	0.2431283	1.1907974
C	-4.2924000	-0.8602092	0.4834670
F	2.6759660	1.4196842	1.1279377
F	-1.4909363	1.8345497	-1.1666963
F	-0.7627221	4.2424842	-2.0141656
F	1.6694207	5.3041607	-1.3179432
F	3.3725341	3.8476377	0.2629905
F	-2.1050533	1.6406121	1.8791470
F	-4.7083360	1.0539457	1.8175108
F	-5.6100205	-1.1373313	0.4359655
F	-3.8114684	-2.7232548	-0.8974847
F	-1.2151352	-2.1733796	-0.8522938
C	1.0825533	-1.1589047	0.2812641
C	2.0012683	-1.1026817	-0.7680607
C	1.0581431	-2.3913249	0.9460426
C	2.8629417	-2.1457226	-1.1059457
C	1.8980529	-3.4569353	0.6455122
C	2.8189462	-3.3328313	-0.3891631
F	0.1464608	-2.6218269	1.9214889
F	1.8174945	-4.6185826	1.3315015
F	3.6422413	-4.3532664	-0.6993108
F	3.7355259	-2.0141853	-2.1298028
F	2.0967656	-0.0042201	-1.5630151
Cl	0.4081472	0.2523999	2.6827212

Bf_3_$OPEt_3$: adduct of $B(C_6F_5)_3$ and $OPEt_3$
57
Energy = -2864.108476470

B	0.0203436	0.0081538	0.0142968
C	0.5543609	1.4689110	-0.5090085
C	0.2102766	2.6297883	0.1878113
C	1.3763563	1.6894328	-1.6140242
C	0.6618642	3.9024816	-0.1380832
C	1.8527410	2.9467001	-1.9839667
C	1.4988212	4.0636018	-1.2378220
C	-1.6080333	-0.1669395	-0.0948456
C	-2.4779914	0.6671660	-0.7970853
C	-2.2407285	-1.2154838	0.5773953
C	-3.8632986	0.5080002	-0.8046679
C	-3.6155122	-1.4140904	0.6035890
C	-4.4401068	-0.5367900	-0.0936724
F	1.7536199	0.6665769	-2.4219300
F	-0.6426821	2.5567918	1.2453106
F	0.2909296	4.9777464	0.5870124
F	1.9485524	5.2835387	-1.5789663
F	2.6514166	3.0896828	-3.0607348
F	-1.4960948	-2.1363620	1.2474299
F	-4.1554654	-2.4452796	1.2852090
F	-5.7736089	-0.7049726	-0.0879956
F	-4.6487829	1.3559965	-1.4986128
F	-2.0099288	1.6972350	-1.5455626
C	0.8465945	-1.2471524	-0.6448874
C	0.3236547	-2.1878436	-1.5318241
C	2.1887343	-1.4544733	-0.3167163
C	1.0477255	-3.2723851	-2.0244327
C	2.9504699	-2.5216671	-0.7774777
C	2.3711198	-3.4471008	-1.6394469
F	2.8397117	-0.5653263	0.4809366
F	4.2405990	-2.6629863	-0.4095479
F	3.0854646	-4.4877313	-2.1020079
F	0.4780702	-4.1519692	-2.8728154
F	-0.9495864	-2.0832258	-1.9898475
P	0.5774898	-0.0844005	3.0175955
O	0.3454944	-0.0324322	1.5120732
C	1.3544722	1.4474798	3.5893898
C	2.6523941	1.7969549	2.8451587
H	1.5304328	1.3305771	4.6657365
H	0.6120408	2.2426103	3.4660461
H	3.4297913	1.0482700	3.0193468
H	2.4795124	1.8665413	1.7685261
H	3.0258224	2.7614576	3.1994272
C	-0.9749761	-0.3033556	3.9231729

C	-2.0240888	0.7849467	3.6494696
H	-0.7099634	-0.3399333	4.9871261
H	-1.3597234	-1.2920746	3.6525755
H	-2.2561634	0.8476893	2.5838264
H	-2.9435892	0.5460201	4.1905047
H	-1.6801814	1.7671356	3.9839920
C	1.6764017	-1.4582748	3.4449881
C	1.1824307	-2.8323789	2.9684682
H	1.7983900	-1.4346879	4.5347956
H	2.6515008	-1.2245684	3.0045771
H	0.2421159	-3.1114077	3.4511048
H	1.0275182	-2.8394371	1.8870867
H	1.9290066	-3.5916652	3.2162872

Bf_3 : borane $B(C_6F_5)_3$
34
Energy = -2209.516695489

B	-0.0026010	-0.0035691	0.0018249
C	0.1623555	1.5511744	0.0033796
C	-0.6758152	2.3951203	-0.7407667
C	1.1616150	2.1982255	0.7459224
C	-0.5331435	3.7761901	-0.7658848
C	1.3190166	3.5776884	0.7665920
C	0.4683494	4.3709175	-0.0009350
C	-1.4315235	-0.6367920	0.0029897
C	-1.7409286	-1.7941438	-0.7281021
C	-2.4950678	-0.0861165	0.7348081
C	-3.0075049	-2.3627849	-0.7495082
C	-3.7681774	-0.6401129	0.7578489
C	-4.0263359	-1.7837358	0.0046546
F	2.0047855	1.4780837	1.5155451
F	-1.6541907	1.8707594	-1.5086662
F	-1.3440697	4.5416687	-1.5133905
F	0.6126223	5.6993454	-0.0033627
F	2.2758772	4.1536711	1.5116466
F	-2.2978002	1.0132976	1.4922200
F	-4.7482491	-0.0902610	1.4923513
F	-5.2482098	-2.3242583	0.0055571
F	-3.2614531	-3.4581265	-1.4830259
F	-0.7954748	-2.3885918	-1.4857259
C	1.2628800	-0.9209785	-0.0021284
C	2.4180657	-0.6014207	-0.7323611
C	1.3246076	-2.1195983	0.7253097
C	3.5483078	-1.4076490	-0.7568721
C	2.4453405	-2.9391400	0.7450391
C	3.5628349	-2.5821464	-0.0070769
F	0.2758153	-2.5069906	1.4810028
F	2.4654381	-4.0656207	1.4750935
F	4.6458687	-3.3645850	-0.0093315
F	4.6216556	-1.0709735	-1.4894964
F	2.4542903	0.5171905	-1.4866014

Cl^- : chloride
1
Energy = -460.3919624889

Cl	0.0000000	0.0000000	0.0000000

Fc : ferrocene
21
Energy = -1651.176296718

Fe	-0.0000073	0.0002369	-0.0000055
C	-0.0001886	1.2195299	1.6307331
C	0.0009376	1.2194385	-1.6307990
C	0.7158842	-0.9866882	1.6306486
C	-0.7165383	-0.9863121	-1.6305967
C	0.7169615	-0.9867990	-1.6301046
C	-0.7176196	-0.9862640	1.6301418
C	1.1603940	0.3764185	-1.6302617
C	-1.1601723	0.3772392	1.6302100
C	1.1592870	0.3765356	1.6309885
C	-1.1590822	0.3771918	-1.6310177
H	0.0001376	2.3012708	1.6052601
H	0.0012986	2.3011798	-1.6053663
H	1.3514728	-1.8620056	1.6049870
H	-1.3526669	-1.8612355	-1.6048832
H	1.3524815	-1.8621538	-1.6039664
H	-1.3537100	-1.8612052	1.6040323
H	2.1893089	0.7103252	-1.6044635
H	-2.1888745	0.7117957	1.6043736
H	2.1882122	0.7104618	1.6058486
H	-2.1877930	0.7117827	-1.6058976

$\mathbf{Fc}^+$: ferrocene radical cation
21
Energy = -1650.993361354

Fe	-0.0000008	-0.0000039	-0.1101766
C	-0.0000138	-1.7634585	-1.3153126
C	0.0000136	1.7634544	-1.3153135
C	0.7180769	-1.6491694	0.8784077
C	-0.7180717	1.6491825	0.8783986
C	0.7181130	1.6491468	0.8784056
C	-0.7181178	-1.6491595	0.8784139
C	1.1535365	1.7178428	-0.4834779
C	-1.1535264	-1.7178833	-0.4834742
C	1.1535017	-1.7178871	-0.4834721
C	-1.1535065	1.7178966	-0.4834723
H	-0.0000010	-1.7651327	-2.3972589
H	-0.0000024	1.7651488	-2.3972597
H	1.3568503	-1.5970916	1.7491922
H	-1.3568469	1.5971245	1.7491776
H	1.3568928	1.5970754	1.7491699
H	-1.3569028	-1.5970919	1.7491784
H	2.1797007	1.6970078	-0.8247519
H	-2.1796919	-1.6970376	-0.8247743
H	2.1796789	-1.6970509	-0.8247364
H	-2.1796821	1.6970869	-0.8247083

HCCPhOMe : alkyne
18
Energy = -423.1805115787

C	4.1481463	-0.3006885	-0.0133508
C	2.9426490	-0.1698092	-0.0031195
H	5.2093738	-0.4166312	-0.0223694
C	1.5270291	-0.0135742	0.0087476
C	0.6782523	-1.1337446	0.0303606
C	0.9421670	1.2713543	-0.0009468
C	-0.7068089	-0.9888930	0.0418635
H	1.1102892	-2.1295943	0.0382819
C	-0.4345145	1.4236772	0.0105687
H	1.5819558	2.1480882	-0.0176772
C	-1.2695049	0.2947210	0.0319653
H	-1.3326028	-1.8734224	0.0583692
H	-0.8853841	2.4113576	0.0033178
O	-2.6108271	0.5446025	0.0417769
C	-3.4962288	-0.5911493	0.0630724
H	-3.3347495	-1.1896282	0.9662833
H	-4.5020668	-0.1724599	0.0672786
H	-3.3510543	-1.2106530	-0.8286661

$OPEt_3$: phosphine oxide
23
Energy = -654.5487161414

P	-0.0001940	-0.3661962	0.1713779
O	-0.0003890	-1.4117988	1.2582403
C	-0.0001628	1.3278685	0.8551744
C	0.0009828	2.4701136	-0.1708999
H	0.8768528	1.3897497	1.5105211
H	-0.8781210	1.3902885	1.5092134
H	-0.8837840	2.4325163	-0.8140834
H	0.0004764	3.4372898	0.3414118
H	0.8871636	2.4324194	-0.8121274
C	1.4455112	-0.4832910	-0.9367206
C	2.7811875	-0.3492668	-0.1908642
H	1.3521648	0.2734981	-1.7248182
H	1.3731485	-1.4639817	-1.4230001
H	2.8446562	-1.0787386	0.6221135
H	3.6182403	-0.5217767	-0.8743719
H	2.8993278	0.6508017	0.2387939
C	-1.4459083	-0.4831919	-0.9367718
C	-2.7815924	-0.3489220	-0.1909596
H	-1.3736914	-1.4639729	-1.4229035
H	-1.3525561	0.2734720	-1.7249912
H	-2.8999677	0.6514664	0.2378745
H	-3.6186262	-0.5222567	-0.8742784
H	-2.8448218	-1.0777729	0.6225985

PPh_3 : less basic phosphine
34
Energy = -1036.779108944

P	0.0578020	-0.0038816	-1.3001914
C	0.6612369	1.5200465	-0.4675093
C	0.3032144	2.7512988	-1.0407071
C	1.4514657	1.5165881	0.6902091
C	0.7078487	3.9512721	-0.4573416
H	-0.2978667	2.7671785	-1.9472345
C	1.8677177	2.7180657	1.2666947
H	1.7400106	0.5722485	1.1421553
C	1.4940775	3.9370817	0.6978665
H	0.4181956	4.8962293	-0.9087250
H	2.4802272	2.7010309	2.1641706
H	1.8177249	4.8711488	1.1484086
C	1.0231146	-1.3077710	-0.4352746
C	0.5485120	-2.0284937	0.6692421
C	2.3087606	-1.5884105	-0.9265861
C	1.3451997	-3.0023955	1.2743082
H	-0.4452112	-1.8259926	1.0576408
C	3.1091697	-2.5515845	-0.3139950
H	2.6833456	-1.0459188	-1.7918693
C	2.6274167	-3.2633753	0.7878852
H	0.9649020	-3.5536248	2.1301429
H	4.1039926	-2.7534065	-0.7015408
H	3.2465293	-4.0206212	1.2606608
C	-1.6059046	-0.2086613	-0.5453766
C	-2.4583269	-1.1674855	-1.1171196
C	-2.0628662	0.5350494	0.5512201
C	-3.7295668	-1.3923566	-0.5907447
H	-2.1208762	-1.7414408	-1.9773656
C	-3.3409451	0.3189512	1.0698828
H	-1.4171330	1.2831797	1.0015389
C	-4.1751494	-0.6467486	0.5039522
H	-4.3755390	-2.1417234	-1.0399533
H	-3.6825064	0.9026544	1.9205057
H	-5.1689463	-0.8144961	0.9094893

$P(tBu)_3H^+$: cation
41
Energy = -815.6863569831

P	-0.0002583	0.0000728	-0.3964387
C	1.6314042	-0.8036127	0.0530277
C	2.8022581	0.1757906	-0.1702778
C	1.6349151	-1.2703826	1.5213429
C	1.8654451	-1.9962988	-0.9034451
H	2.8484268	0.5321792	-1.2026839
H	2.7785762	1.0283680	0.5096615
H	3.7223328	-0.3832024	0.0312303
H	0.8843214	-2.0387007	1.7166716
H	2.6180467	-1.7051942	1.7302774
H	1.4806713	-0.4421600	2.2174452
H	2.8747897	-2.3732565	-0.7065249
H	1.1677535	-2.8167875	-0.7488931
H	1.8219184	-1.6828362	-1.9508888
C	-1.5118410	-1.0114580	0.0531225
C	-1.2490680	-2.5151276	-0.1705151
C	-1.9170345	-0.7811903	1.5216381
C	-2.6619993	-0.6177154	-0.9029109
H	-0.9644100	-2.7331753	-1.2031895
H	-0.4981976	-2.9208597	0.5086960
H	-2.1929682	-3.0324988	0.0318817
H	-2.2079227	0.2527805	1.7168131
H	-2.7842659	-1.4161076	1.7314095

H	-1.1218167	-1.0607090	2.2172055
H	-3.4933481	-1.3028522	-0.7052830
H	-3.0231813	0.3970258	-0.7487945
H	-2.3692192	-0.7373253	-1.9504129
C	-0.1197491	1.8151105	0.0533320
C	-1.5532954	2.3394972	-0.1707539
C	0.2822226	2.0514955	1.5217292
C	0.7965296	2.6138637	-0.9029281
H	-1.8841294	2.2018299	-1.2035931
H	-2.2804105	1.8921066	0.5081459
H	-1.5294974	3.4156284	0.0314381
H	1.3220393	1.7833166	1.7180283
H	0.1694848	3.1206916	1.7297661
H	-0.3597039	1.5057591	2.2176242
H	0.6178512	3.6764708	-0.7066318
H	1.8558641	2.4202152	-0.7475647
H	0.5476704	2.4188483	-1.9504515
H	-0.0002045	0.0004005	-1.7999231

P(*t*Bu)$_3$: strong basic phosphine
40
Energy = -815.2249339339

P	0.0001537	0.0001221	-0.6859747
C	1.7823025	0.1080241	0.0205435
C	2.3199069	1.5376016	-0.1938672
C	1.9864304	-0.2698352	1.4971566
C	2.6720996	-0.7953046	-0.8657493
H	2.1835844	1.8674954	-1.2291520
H	1.8562832	2.2677563	0.4724387
H	3.3970546	1.5329402	0.0181594
H	1.7466415	-1.3177620	1.6916238
H	3.0433061	-0.1211811	1.7594419
H	1.3857804	0.3494687	2.1670187
H	3.7217157	-0.6362992	-0.5841121
H	2.4539948	-1.8569822	-0.7504495
H	2.5577287	-0.5337658	-1.9229769
C	-0.7972375	-1.5971996	0.0206152
C	0.1721419	-2.7774330	-0.1932640
C	-1.2274600	-1.5852492	1.4970494
C	-2.0241874	-1.9165632	-0.8659449
H	0.5264058	-2.8243745	-1.2283554
H	1.0358859	-2.7409874	0.4734860
H	-0.3705807	-3.7079786	0.0184903
H	-2.0162433	-0.8545254	1.6908053
H	-1.6262906	-2.5752790	1.7592085
H	-0.3916458	-1.3735681	2.1674802
H	-2.4118331	-2.9047386	-0.5835552
H	-2.8344795	-1.1965696	-0.7515060
H	-1.7400869	-1.9493751	-1.9230013
C	-0.9848074	1.4893163	0.0205022
C	-2.4915186	1.2396872	-0.1938782
C	-0.7596749	1.8553818	1.4970995
C	-0.6476681	2.7117416	-0.8656298
H	-2.7090647	0.9568258	-1.2291598
H	-2.8916817	0.4729458	0.4724088
H	-3.0263043	2.1746769	0.0183835
H	0.2675513	2.1730678	1.6911426
H	-1.4178237	2.6955376	1.7595266
H	-0.9940679	1.0252774	2.1670793
H	-1.3097829	3.5413866	-0.5833778
H	0.3810098	3.0534145	-0.7507341
H	-0.8175383	2.4823037	-1.9228694

P(To)$_3$H$^+$: cation
44
Energy = -1155.246375121

P	-1.7816918	-1.1123808	0.0411304
C	-1.2154254	-1.7208818	1.6287086
C	-2.9734205	-2.2260314	-0.6980017
C	-2.3687922	0.5777992	0.0827563
C	-1.9225766	-2.7642381	2.2442901
C	-0.0934198	-1.1262438	2.2490654
C	-4.2843684	-1.7668158	-0.8983419
C	-2.5836737	-3.5301244	-1.0836465
C	-3.2843344	1.0401773	1.0545083
C	-1.8655887	1.4336480	-0.9122062
C	-1.5206012	-3.2367076	3.4885126
H	-2.7858287	-3.1993284	1.7492527
C	0.2895198	-1.6262431	3.4976472
C	0.6659954	0.0091831	1.6147731
C	-5.2365404	-2.6078192	-1.4649973
H	-4.5516085	-0.7511170	-0.6239734
C	-3.5621556	-4.3473371	-1.6579122
C	-1.1794412	-4.0429996	-0.8990124
C	-3.6727421	2.3818487	0.9796393
C	-3.8276944	0.1619973	2.1520522
C	-2.2709968	2.7628674	-0.9583930
H	-1.1567240	1.0572502	-1.6442484
C	-0.4108089	-2.6642614	4.1126917
H	-2.0675198	-4.0438041	3.9646173
H	1.1520401	-1.1893986	3.9931701
H	1.0008495	-0.2431344	0.6012089
H	0.0441956	0.9090547	1.5407310
H	1.5493807	0.2563088	2.2067830
C	-4.8713438	-3.9010408	-1.8404597
H	-6.2500969	-2.2525648	-1.6186221
H	-3.2861697	-5.3503216	-1.9713194
H	-0.4306871	-3.3023993	-1.2036318
H	-0.9835607	-4.2964516	0.1491449
H	-1.0222571	-4.9429751	-1.4970886
C	-3.1770922	3.2339214	-0.0072842
H	-4.3800775	2.7609634	1.7119227
H	-4.1065852	-0.8319711	1.7873413
H	-3.0839562	0.0223375	2.9446676
H	-4.7142812	0.6188888	2.5970079
H	-1.8820475	3.4221470	-1.7273490
H	-0.0875994	-3.0272455	5.0836259
H	-5.6057435	-4.5637410	-2.2881680
H	-3.5008553	4.2699900	-0.0327767
H	-0.6675825	-1.0521944	-0.8061870

$P(To)_3$: less basic phosphine
43
Energy = -1154.805466726

P	-1.4424738	-1.0994628	-0.1877858
C	-1.3698371	-1.6113284	1.5750357
C	-2.7579772	-2.1868495	-0.8674776
C	-2.2785497	0.5338524	-0.0973881
C	-2.2448273	-2.5676490	2.1095563
C	-0.3524563	-1.0661023	2.3933505
C	-4.0556468	-1.7185545	-1.1182359
C	-2.4225097	-3.5191587	-1.2055895
C	-2.3809475	1.3045124	-1.2795378
C	-2.7535862	1.0613209	1.1117735
C	-2.1255044	-2.9933167	3.4318865
H	-3.0280572	-2.9815407	1.4809939
C	-0.2511285	-1.5016533	3.7196723
C	0.5915326	-0.0132329	1.8724091
C	-5.0187966	-2.5429095	-1.6985909
H	-4.3118474	-0.6965286	-0.8546461
C	-3.4041907	-4.3339594	-1.7813887
C	-1.0493457	-4.0752249	-0.9295681
C	-2.9553149	2.5786599	-1.2035385
C	-1.9168169	0.7660067	-2.6083437
C	-3.3188182	2.3345959	1.1691390
H	-2.6791655	0.4657110	2.0170485
C	-1.1232837	-2.4578552	4.2410645
H	-2.8134294	-3.7360585	3.8264251
H	0.5310258	-1.0847200	4.3503475
H	0.9467248	-0.2676681	0.8665135
H	0.0883516	0.9587376	1.7934991
H	1.4528283	0.1030651	2.5357597
C	-4.6914205	-3.8573372	-2.0319179
H	-6.0181685	-2.1600290	-1.8862854
H	-3.1491472	-5.3591965	-2.0404981
H	-0.2707217	-3.3567261	-1.2127697
H	-0.9176938	-4.2787877	0.1406792
H	-0.8882453	-5.0089438	-1.4750947
C	-3.4199753	3.0973304	0.0055563
H	-3.0325305	3.1741939	-2.1105757
H	-0.9441289	0.2686962	-2.5121791
H	-2.6189560	0.0156217	-2.9932945
H	-1.8362200	1.5666489	-3.3485440
H	-3.6791944	2.7255421	2.1166759
H	-1.0182663	-2.7826814	5.2726077
H	-5.4324157	-4.5094186	-2.4861838
H	-3.8566317	4.0918137	0.0370897

TS0a : chloride abstraction
71
Energy = -3479.491134933

C	0.1983233	-0.1245180	-2.5843536
C	-0.0922782	0.7560306	-3.6943068
C	1.1923067	0.5841608	-3.3627337
C	-0.0461641	-1.5821393	-2.4466209
C	-1.1391399	1.3828425	-4.4479001
C	2.5884935	0.8803514	-3.4971080
C	-1.2378444	-2.1359979	-2.9313155
C	0.9349862	-2.4303167	-1.9171896
C	-2.4692809	1.2877331	-3.9956961
C	-0.8596982	2.1115366	-5.6196804
C	3.0745529	1.6096401	-4.5997162
C	3.4879657	0.4577284	-2.4999801
C	-1.4399403	-3.5150845	-2.8996111
H	-2.0004561	-1.4864707	-3.3489000
C	0.7300498	-3.8075910	-1.8795317
H	1.8602232	-2.0115234	-1.5407803
H	-2.6775127	0.7480140	-3.0768631
C	-3.4951615	1.9077858	-4.7008172
H	0.1629959	2.1865952	-5.9752342
C	-1.8918411	2.7192158	-6.3264497
H	2.3870854	1.9376480	-5.3727914
C	4.4309066	1.8983177	-4.7021028
H	3.1087851	-0.0849081	-1.6411747
C	4.8416287	0.7602948	-2.6026615
C	-0.4565202	-4.3545606	-2.3741018
H	-2.3662959	-3.9330462	-3.2817430
H	1.4997565	-4.4560509	-1.4708148
C	-3.2099369	2.6200355	-5.8693734
H	-4.5179598	1.8371165	-4.3430275
H	-1.6711275	3.2738044	-7.2335412
H	4.8007404	2.4555310	-5.5575543
C	5.3167435	1.4764954	-3.7048492
H	5.5275171	0.4383900	-1.8249573
H	-0.6150094	-5.4285444	-2.3456825
H	-4.0126282	3.0991008	-6.4221268
H	6.3746780	1.7075345	-3.7868300
Cl	-0.1715765	0.7543593	-0.8182770
B	-0.3023508	-0.0430083	1.8597200
C	-0.5704135	-1.5590153	1.5314595
C	-1.5259942	0.9146300	2.1497287
C	1.1504831	0.4688212	2.2045059
C	-1.6778021	-1.9820993	0.7765308
C	0.2348170	-2.5968741	2.0221011
C	-2.7101937	0.4658427	2.7507724
C	-1.5030542	2.2853721	1.8506881
C	2.2923815	0.0587997	1.5020190
C	1.4004185	1.3783134	3.2427922
F	-2.5352129	-1.0819176	0.2584862
C	-1.9689256	-3.3154729	0.5266051
F	1.3015950	-2.3287304	2.8083899
C	-0.0168882	-3.9426402	1.7803296
F	-2.8318535	-0.8197021	3.1517331
C	-3.8018726	1.2880501	3.0049667
F	-0.3991599	2.8492858	1.3199430
C	-2.5800640	3.1347211	2.0697201
F	2.1898458	-0.8493842	0.5108695
C	3.5682900	0.5413802	1.7587481
F	0.3948927	1.8080942	4.0370447
C	2.6659393	1.8679875	3.5470764

F	-3.0596265	-3.6631632	-0.1775417
C	-1.1271012	-4.3047433	1.0263401
F	0.7960423	-4.8953497	2.2737077
F	-4.9100657	0.8003133	3.5908274
C	-3.7410102	2.6321293	2.6511046
F	-2.5085847	4.4376247	1.7421207
F	4.6217836	0.1241386	1.0321899
C	3.7587032	1.4553104	2.7916146
F	2.8438545	2.7311611	4.5626529
F	-1.3871851	-5.5963856	0.7855558
F	-4.7845260	3.4397949	2.8813750
F	4.9842698	1.9199184	3.0644895

TS0 : chloride abstraction

61

Energy = -3248.291268509

H	-0.0904939	-1.0148909	-1.9163162
C	-0.0551573	-0.0405908	-2.3887897
C	-0.7236853	0.4773641	-3.5539695
C	0.6133460	0.4022277	-3.5841303
C	-1.9965005	0.7966114	-4.1326468
C	1.8925832	0.5852141	-4.2058149
C	-3.1692983	0.6099835	-3.3769023
C	-2.0915711	1.2954196	-5.4462212
C	2.0048134	1.1301796	-5.4994162
C	3.0579956	0.2210915	-3.5048820
H	-3.0922720	0.2365022	-2.3615036
C	-4.4104346	0.9148920	-3.9262494
H	-1.1905085	1.4408286	-6.0334069
C	-3.3359096	1.5930308	-5.9903118
H	1.1103410	1.4181441	-6.0424213
C	3.2581614	1.3001883	-6.0770336
H	2.9655364	-0.1976933	-2.5088525
C	4.3084978	0.3973247	-4.0877052
C	-4.4966446	1.4046354	-5.2325080
H	-5.3123223	0.7722048	-3.3385987
H	-3.4044500	1.9744650	-7.0045961
H	3.3400913	1.7191407	-7.0753770
C	4.4112266	0.9355681	-5.3736333
H	5.2044440	0.1164787	-3.5421266
H	-5.4664994	1.6410404	-5.6600747
H	5.3881485	1.0723598	-5.8277729
F	-2.5380323	-0.3195791	-0.0313570
C	-1.8648426	-1.4788747	0.1324334
C	-0.6338511	-1.4906345	0.8050616
C	-2.4610118	-2.6130495	-0.4035684
C	-0.0646294	-2.7621935	0.9547354
B	0.0307217	-0.1680382	1.3797340
F	-3.6314001	-2.5301004	-1.0614845
C	-1.8415837	-3.8502447	-0.2445707
F	1.0865381	-2.9256565	1.6429141
C	-0.6387223	-3.9252458	0.4492302
C	-0.8870111	0.8588299	2.1674997
C	1.5996024	-0.1249676	1.6102446
Cl	0.0687124	1.1529639	-0.8100060
F	-2.4065988	-4.9570412	-0.7423131
F	-0.0456926	-5.1178001	0.6303191
C	-2.0376950	0.4683717	2.8640595
C	-0.5887820	2.2259896	2.2518106
C	2.5099799	-0.6059087	0.6596548
C	2.1906298	0.3823410	2.7746141
F	-2.4052398	-0.8327424	2.9153513
C	-2.8490156	1.3554895	3.5646954
F	0.5225508	2.7140638	1.6581307
C	-1.3800383	3.1460286	2.9264956
F	2.0598172	-1.1696954	-0.4848180
C	3.8880359	-0.5432689	0.8072243
F	1.4291561	0.8207413	3.8017795
C	3.5673186	0.4454014	2.9718554
F	-3.9391072	0.9182684	4.2206380
C	-2.5231617	2.7069486	3.5894667
F	-1.0484985	4.4492138	2.9586142
F	4.7065571	-1.0011506	-0.1584292
C	4.4244744	-0.0106884	1.9768608
F	4.0743672	0.9405502	4.1146843
F	-3.2938771	3.5771133	4.2554303
F	5.7517774	0.0475216	2.1460692

TS1^{+} : alkyne addition to **2**$^{+}$

54

Energy = -1232.718640043

C	-1.8128911	-1.9939008	-0.2582452
C	-3.1722745	-2.3017913	-0.4107700
C	-0.8535859	-3.0050451	-0.4202335
C	-1.4066392	-0.6098522	0.0416810
H	-3.9206939	-1.5251159	-0.2899839
C	-3.5618507	-3.5979621	-0.7450930
H	0.1969798	-2.7757606	-0.2713769
C	-1.2454635	-4.2982499	-0.7484686
C	-1.9316563	0.7004508	-0.1854656
C	-0.6898186	0.4261324	-0.6397076
C	-2.6017713	-4.5972827	-0.9125938
H	-4.6155037	-3.8260411	-0.8734549
H	-0.4971969	-5.0745354	-0.8758332
C	-3.0317057	1.5938185	0.0147379
C	0.5171313	0.8127898	-1.3073625
H	-2.9074690	-5.6075350	-1.1671035
C	-4.1303530	1.1888548	0.7984623
C	-3.0233863	2.8838478	-0.5526735
C	0.7470227	2.1616064	-1.6429603
C	1.5006558	-0.1496867	-1.6076550
H	-4.1363930	0.1994263	1.2448632
C	-5.1943659	2.0577002	1.0113991
H	-2.1833440	3.1986966	-1.1626609
C	-4.0958103	3.7423543	-0.3448188
H	-0.0011688	2.9102066	-1.4053510
C	1.9382173	2.5350652	-2.2538567
H	1.3262524	-1.1879776	-1.3488547
C	2.6857194	0.2293106	-2.2240569
C	-5.1804534	3.3326780	0.4380839

H	-6.0356107	1.7432929	1.6209329
H	-4.0888078	4.7326178	-0.7893050
H	2.1138482	3.5770403	-2.5020793
C	2.9084090	1.5716568	-2.5460423
H	3.4392373	-0.5180645	-2.4523532
H	-6.0147328	4.0081547	0.6013065
H	3.8379849	1.8673368	-3.0227238
C	-0.9292367	-0.8148640	1.9678037
C	0.3018030	-0.6714718	2.0725552
H	-1.8474060	-1.0004160	2.4938264
C	1.6515797	-0.4148216	1.8642060
C	2.5628300	-1.4689818	1.6113392
C	2.1128444	0.9288526	1.7908935
C	3.8671192	-1.2015787	1.2436048
H	2.2217165	-2.4959201	1.6910854
C	3.4079537	1.1986356	1.4190475
H	1.4212545	1.7377668	1.9994040
C	4.2919081	0.1378756	1.1250304
H	4.5467879	-2.0199353	1.0409450
H	3.7684611	2.2179626	1.3320202
O	5.5246335	0.5023828	0.7336020
C	6.4781205	-0.5362350	0.4001470
H	6.1032631	-1.1386461	-0.4324842
H	7.3818819	-0.0053924	0.1073229
H	6.6722444	-1.1653537	1.2732855

TS2^{+}o : alkyne deprotonation with P(To)$_3$
97
Energy = -2387.552354010

C	0.2418306	-1.7682837	-2.3057031
C	-0.3540507	-1.7426355	-3.5740841
C	0.1150611	-2.9257615	-1.5271579
C	0.9839187	-0.5656055	-1.7881664
H	-0.2587486	-0.8537974	-4.1919905
C	-1.0758554	-2.8396959	-4.0418536
H	0.5863746	-2.9646209	-0.5492321
C	-0.6067316	-4.0247778	-1.9932439
C	1.0317090	0.7136250	-2.5828635
C	2.1561160	0.0320996	-2.5151537
C	-1.2107952	-3.9832804	-3.2501265
H	-1.5411792	-2.7983765	-5.0226500
H	-0.6993657	-4.9112515	-1.3723124
C	0.2169382	1.7971677	-3.0522064
C	3.5426998	-0.2127694	-2.7715786
H	-1.7818151	-4.8334969	-3.6113956
C	-1.1851927	1.7082131	-2.9676342
C	0.7971922	2.9518823	-3.6115280
C	4.3237321	0.6951651	-3.5146852
C	4.1429310	-1.3800897	-2.2613129
H	-1.6316435	0.8182770	-2.5362723
C	-1.9864980	2.7392822	-3.4423218
H	1.8783106	3.0337553	-3.6696077
C	-0.0099253	3.9874936	-4.0707913
H	3.8664578	1.5959593	-3.9123909
C	5.6710202	0.4352485	-3.7391168
H	3.5384524	-2.0790670	-1.6907948
C	5.4925467	-1.6319240	-2.4876914
C	-1.4019428	3.8830531	-3.9918555
H	-3.0668255	2.6586366	-3.3765079
H	0.4451812	4.8786062	-4.4931223
H	6.2673510	1.1377545	-4.3138839
C	6.2592597	-0.7263412	-3.2260556
H	5.9489952	-2.5338061	-2.0907315
H	-2.0284080	4.6928499	-4.3537787
H	7.3124815	-0.9237640	-3.4026276
C	0.9739063	-0.4755616	-0.2855459
C	1.7475320	-0.4532726	0.7042633
H	-0.2551856	-0.3556902	0.0694757
C	2.4386782	-0.4043410	1.9072885
C	2.8554318	-1.5989993	2.5462260
C	2.7342450	0.8389993	2.5317205
C	3.5314999	-1.5638992	3.7517084
H	2.6358523	-2.5526320	2.0776561
C	3.4011794	0.8769058	3.7349699
H	2.4178070	1.7603199	2.0545957
C	3.8053405	-0.3223237	4.3566680
H	3.8389106	-2.4909161	4.2199624
H	3.6213336	1.8195743	4.2252103
O	4.4441189	-0.1817398	5.5370849
C	4.8645718	-1.3780615	6.2332084
H	5.5614533	-1.9525641	5.6156691
H	5.3630833	-1.0216142	7.1331326
H	3.9947618	-1.9877299	6.4969474
P	-1.8693194	0.1060430	0.7182907
C	-1.3223618	0.0563321	2.4401900
C	-1.2311464	1.2345177	3.1980407
C	-0.8395368	-1.1658837	2.9619399
C	-0.6545309	1.2177167	4.4631736
H	-1.6067721	2.1665851	2.7889134
C	-0.2638208	-1.1554272	4.2365975
C	-0.1605577	0.0186817	4.9792622
H	-0.5850711	2.1356288	5.0386134
H	0.1235888	-2.0863512	4.6418578
H	0.3073072	-0.0012896	5.9590352
C	-2.1345674	1.8401528	0.2724386
C	-3.3528961	2.4658855	-0.0751258
C	-0.9308013	2.5735632	0.2295626
C	-3.3055445	3.8217339	-0.4279595
C	-0.9155553	3.9174505	-0.1178588
H	0.0042885	2.0724423	0.4671573
C	-2.1157264	4.5451689	-0.4491490
H	-4.2358093	4.3154686	-0.6968483
H	0.0233791	4.4607757	-0.1483869
H	-2.1254225	5.5922848	-0.7360398
C	-3.2616866	-0.9967227	0.3946953
C	-4.2815722	-1.3097518	1.3219109
C	-3.2460070	-1.5948966	-0.8778862
C	-5.2669490	-2.2173558	0.9166435
C	-4.2464314	-2.4827451	-1.2588496
H	-2.4336202	-1.3737801	-1.5649797

C	-5.2596559	-2.7958130	-0.3529320
H	-6.0639884	-2.4649580	1.6131122
H	-4.2242941	-2.9331676	-2.2458829
H	-6.0451494	-3.4923585	-0.6311259
C	-0.9424448	-2.4601635	2.1993589
H	-0.2041901	-3.1799096	2.5621917
H	-1.9360258	-2.9092152	2.3167709
H	-0.7863978	-2.3155107	1.1255493
C	-4.6876380	1.7655031	-0.0975767
H	-4.7031987	0.9470005	-0.8239795
H	-4.9378604	1.3376565	0.8769846
H	-5.4729501	2.4760897	-0.3660219
C	-4.3586163	-0.7071886	2.7009690
H	-5.3652861	-0.8278512	3.1085385
H	-3.6561488	-1.1942030	3.3872013
H	-4.1098487	0.3579803	2.6983857

TS2^{+} : alkyne deprotonation with P(*t*Bu)$_3$

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Energy = -2047.980686856

C	-1.4947400	-1.7821626	-1.2334870
C	-2.7650064	-1.8885325	-1.8145678
C	-0.9937972	-2.8689961	-0.5062017
C	-0.6648059	-0.5455507	-1.4286546
H	-3.1607417	-1.0554909	-2.3898368
C	-3.5213966	-3.0492182	-1.6605613
H	-0.0059208	-2.8010827	-0.0588344
C	-1.7460946	-4.0344751	-0.3562893
C	-1.1289741	0.6001733	-2.2915636
C	-0.1819514	-0.1585353	-2.8003138
C	-3.0158678	-4.1262253	-0.9281712
H	-4.5085428	-3.1119071	-2.1096955
H	-1.3409667	-4.8694307	0.2087293
C	-2.0258952	1.7196969	-2.3490711
C	0.7951594	-0.5424858	-3.7723212
H	-3.6062263	-5.0296390	-0.8067270
C	-3.1042866	1.8082380	-1.4506430
C	-1.8453851	2.7410158	-3.3028974
C	0.9771892	0.1890392	-4.9633242
C	1.6044149	-1.6689659	-3.5263918
H	-3.2506666	1.0135188	-0.7271374
C	-3.9812608	2.8870357	-1.5030183
H	-1.0108687	2.6861245	-3.9951158
C	-2.7216992	3.8201623	-3.3472983
H	0.3547064	1.0562468	-5.1609807
C	1.9453333	-0.2020614	-5.8812446
H	1.4599002	-2.2326996	-2.6097130
C	2.5738876	-2.0519618	-4.4478611
C	-3.7918438	3.8972343	-2.4495103
H	-4.8135685	2.9424165	-0.8073237
H	-2.5716144	4.6057339	-4.0820456
H	2.0795233	0.3644528	-6.7980197
C	2.7465386	-1.3207506	-5.6263389
H	3.1945340	-2.9211799	-4.2513582
H	-4.4744952	4.7408068	-2.4889825
H	3.5025754	-1.6208911	-6.3458740
C	0.2701951	-0.2393917	-0.2792862
C	1.5083388	-0.0304796	-0.1671497
H	-0.3494060	-0.1700545	0.8285873
C	2.8207580	0.2659174	0.1493402
C	3.7365578	-0.7658638	0.4880754
C	3.2822598	1.6149433	0.1502033
C	5.0430692	-0.4745549	0.8256071
H	3.3951580	-1.7956446	0.4843042
C	4.5823072	1.9077293	0.4876172
H	2.5925172	2.4092012	-0.1143082
C	5.4748640	0.8680552	0.8311370
H	5.7232471	-1.2773803	1.0821105
H	4.9450297	2.9302435	0.4966094
O	6.7229184	1.2548036	1.1480290
C	7.6910737	0.2372790	1.5042594
H	7.8535935	-0.4391165	0.6603150
H	8.6032653	0.7850548	1.7328707
H	7.3503350	-0.3172574	2.3832575
P	-1.1677665	0.0200398	2.5327626
C	0.1518318	-0.7855169	3.6384780
C	1.4399549	0.0628377	3.6643712
C	-0.2993153	-1.0233664	5.0909008
C	0.5467370	-2.1284350	2.9808542
H	1.8271119	0.2532315	2.6608834
H	1.3151047	1.0133743	4.1844768
H	2.1986474	-0.5138445	4.2067397
H	-1.1367607	-1.7199480	5.1589430
H	0.5420664	-1.4632524	5.6409478
H	-0.5777727	-0.0933705	5.5913067
H	1.3311578	-2.5889078	3.5931277
H	-0.2794648	-2.8340465	2.9075098
H	0.9528555	-1.9643552	1.9783860
C	-2.8662129	-0.7781255	2.8342462
C	-2.7307327	-2.3125016	2.8826343
C	-3.5619939	-0.2964774	4.1207569
C	-3.7575737	-0.4718326	1.6109248
H	-2.2558791	-2.7036286	1.9794931
H	-2.1877133	-2.6649652	3.7608363
H	-3.7443165	-2.7276440	2.9320860
H	-3.7926876	0.7702770	4.0933826
H	-4.5119671	-0.8375317	4.2142961
H	-2.9693410	-0.5023472	5.0141067
H	-4.6999781	-1.0185738	1.7341703
H	-3.9991630	0.5861848	1.5143206
H	-3.2873329	-0.8228402	0.6879713
C	-1.2347664	1.8921733	2.8459141
C	-2.5051982	2.4960227	2.2169267
C	-1.1912804	2.2877036	4.3335179
C	-0.0473787	2.5340126	2.0902560
H	-2.5887448	2.2498489	1.1557705
H	-3.4191932	2.1938638	2.7306266
H	-2.4252890	3.5866632	2.2974593
H	-0.2537086	2.0045825	4.8151977
H	-1.2794966	3.3794790	4.3982503

H	-2.0176550	1.8505702	4.8979903
H	-0.0908189	3.6177955	2.2509202
H	0.9251184	2.1847506	2.4351385
H	-0.1238322	2.3479563	1.0148593

TS3^{+} : addition of P(tBu)$_3$

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Energy = -2047.985951613

C	-3.0477211	-1.1311270	-1.4608854
C	-3.9219586	-0.6890529	-2.4636791
C	-3.4052716	-2.2502766	-0.6986247
C	-1.7469044	-0.4235843	-1.2268575
H	-3.6521021	0.1756297	-3.0642624
C	-5.1283091	-1.3477200	-2.6923625
H	-2.7308153	-2.6155074	0.0724415
C	-4.6143493	-2.9108137	-0.9267374
C	-1.4203467	0.8940082	-1.8864450
C	-0.7921844	-0.1565707	-2.3608539
C	-5.4804204	-2.4612503	-1.9240398
H	-5.7964939	-0.9895195	-3.4707902
H	-4.8750772	-3.7781073	-0.3267742
C	-1.6666056	2.2926784	-1.7014056
C	0.1563724	-0.8357078	-3.1970076
H	-6.4209901	-2.9738352	-2.1041603
C	-2.5901993	2.7051900	-0.7249997
C	-0.9740845	3.2654006	-2.4433136
C	1.0832079	-0.1308785	-3.9898410
C	0.1858122	-2.2427217	-3.1973061
H	-3.1271690	1.9551172	-0.1546453
C	-2.8114731	4.0581629	-0.4922873
H	-0.2614553	2.9562504	-3.1997292
C	-1.2014654	4.6161318	-2.2060282
H	1.0759219	0.9539610	-3.9852732
C	2.0196636	-0.8220923	-4.7548797
H	-0.5257864	-2.7830908	-2.5794438
C	1.1178847	-2.9273062	-3.9716592
C	-2.1190068	5.0159344	-1.2324531
H	-3.5263953	4.3648234	0.2629051
H	-0.6625560	5.3604278	-2.7816608
H	2.7370220	-0.2722710	-5.3575815
C	2.0393048	-2.2198222	-4.7499501
H	1.1314862	-4.0124261	-3.9663473
H	-2.2915531	6.0719898	-1.0517923
H	2.7687248	-2.7551986	-5.3525870
C	-1.2062310	-0.5582728	0.1969841
C	0.0856675	-0.5888418	0.3858445
H	-1.9186069	-0.5206364	1.0014942
C	1.3641016	-0.4931760	-0.1227127
C	2.1201349	-1.6527881	-0.4343763
C	1.8683788	0.7812287	-0.5291389
C	3.2683358	-1.5671452	-1.1945857
H	1.7562850	-2.6208823	-0.1067040
C	3.0138708	0.8700071	-1.2798405
H	1.3071850	1.6721425	-0.2749263
C	3.7104161	-0.3049301	-1.6457750
H	3.8064788	-2.4674709	-1.4572891
H	3.3898534	1.8267509	-1.6268961
O	4.7765571	-0.1205994	-2.4370262
C	5.5183614	-1.2816677	-2.8922666
H	4.8593832	-1.9424667	-3.4604633
H	6.3021604	-0.8774614	-3.5299049
H	5.9542076	-1.8082263	-2.0400052
P	0.3981686	-0.0710478	3.1801142
C	2.2625226	0.0300991	3.5871947
C	2.8783140	1.2722178	2.9103059
C	2.5981942	0.0670688	5.0879501
C	2.9583438	-1.1918835	2.9390636
H	2.6709025	1.2905049	1.8372029
H	2.5365475	2.2093134	3.3550349
H	3.9675685	1.2239958	3.0404804
H	2.2909217	-0.8477431	5.5993327
H	3.6862325	0.1571202	5.2025317
H	2.1357688	0.9179528	5.5920182
H	4.0424142	-1.0571584	3.0459041
H	2.6914411	-2.1368957	3.4109443
H	2.7258323	-1.2571380	1.8734798
C	-0.4203624	-1.3132394	4.3815694
C	0.4070264	-2.6116389	4.4188773
C	-0.6221845	-0.8085626	5.8196099
C	-1.7799162	-1.7058567	3.7673367
H	0.5864894	-3.0018931	3.4129340
H	1.3625948	-2.4871162	4.9273555
H	-0.1682122	-3.3636071	4.9745345
H	-1.2979611	0.0453838	5.8689017
H	-1.0654688	-1.6207556	6.4127327
H	0.3210870	-0.5301324	6.2865533
H	-2.2358980	-2.4923272	4.3835065
H	-2.4884585	-0.8873421	3.6821666
H	-1.5760798	-2.1203654	2.7854646
C	-0.3833486	1.6524741	3.4490409
C	-1.9169163	1.5300870	3.5295908
C	0.1155667	2.3998398	4.6963288
C	-0.1025277	2.5036474	2.1878762
H	-2.2889240	1.0222184	2.6379110
H	-2.2675112	1.0134196	4.4242084
H	-2.3315498	2.5437891	3.5397197
H	1.1794233	2.6278168	4.6350642
H	-0.4220689	3.3525295	4.7727878
H	-0.0647558	1.8374702	5.6150294
H	-0.6293080	3.4587916	2.2946875
H	0.9545991	2.7208295	2.0367844
H	-0.4918897	2.0034568	1.2973247

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