Supporting Information

Catalytic aerobic photooxidation of triarylphosphines using dibenzo-fused 1,4-azaborines

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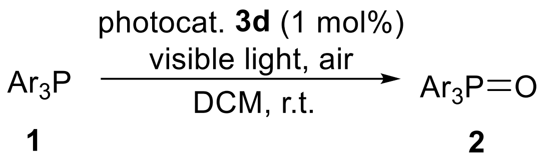
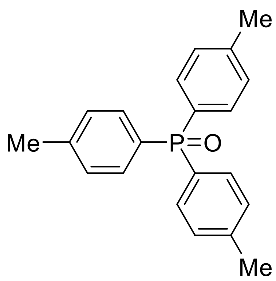
General methods

^{1}H-, ^{13}C-, ^{19}F-, ^{31}P-NMR spectra were recorded with a Bruker AVANCE III (^{1}H-NMR 400 MHz, ^{13}C-NMR 100 MHz, ^{31}P-NMR 160 MHz, and ^{19}F-NMR 376 MHz). ^{1}H-NMR spectra are reported as follows: chemical shift in ppm relative to the chemical shift of $CHCl_3$ at 7.26 ppm and the central line of triplet for CH_2Cl_2 at 5.32 ppm, integration, multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), and coupling constants (Hz). ^{13}C-NMR spectra reported in ppm relative to the central line of triplet for $CDCl_3$ at 77 ppm and quintet for CD_2Cl_2 at 53.84 ppm. ^{31}P-NMR and ^{19}F-NMR spectra were reported in ppm relative to the resonances of 85% H_3PO_4 (0 ppm) and CF_3COOH (–76.55 ppm), respectively. HRMS were recorded on a Bruker timsTOF (IMS-QTOF) spectrometer using the APCI method. Cyclic voltammetry was carried out on a Satoda Science CV-100. UV/vis spectra were recorded on a Shimadzu UV-3101PC spectrophotometer. Kessil 160WE TUNA SUN LED was used as a light source. TOPLAND SF-DF10 BR was used as a fan. Photocatalysts **3a**,[1] **3b**,[2] **3c**,[2] and **3d**[3] were prepared by the reported procedures. IR spectra were recorded on Shimadzu IR Affinity-1. Column chromatography on SiO_2 was performed with Kanto Silica Gel 60 (40-100 μm). Commercially available organic and inorganic compounds were used without further purification.

General procedure for the photooxidation of triarylphosphine 1 with 3d



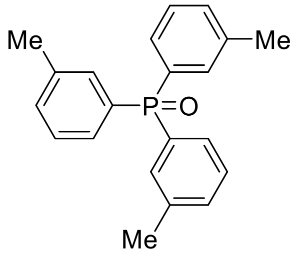
Triarylphosphine **1** (0.2 mmol), DBAB **3d** (1.2 mg, 2 μmol), and DCM (2.0 mL) were added to a screw vial with a stir bar. The mixture was irradiated by a white LED at room temperature under air atmosphere. After completion of the reaction (typically 8 h), the solvent was removed, and the residue was purified by flash column chromatography on silica gel (Hexane/AcOEt = 1/1) to afford **2** as a solid.



2a

2a: 90% yield; white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, J = 8.0, 2.0 Hz, 6H), 7.23 (dd, J = 8.0, 2.0 Hz, 6H), 2.37 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 142.1 (d, $J_{C\text{-}P}$ = 3.0 Hz), 132.0 (d, $J_{C\text{-}P}$ = 10 Hz), 129.7 (d, $J_{C\text{-}P}$ = 105 Hz), 129.1 (d, $J_{C\text{-}P}$ = 12 Hz), 21.5; ^{31}P-NMR (160 MHz, $CDCl_3$) δ 29.2.

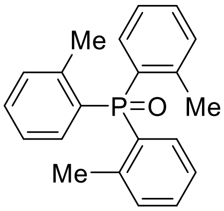
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[4]



2b

2b: 92% yield; white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 11.6 Hz, 3H), 7.38-7.33 (m, 9H), 2.36 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 138.4 (d, J_{C-P} = 11 Hz), 129.2 (d, J_{C-P} = 6 Hz), 128.2 (d, J_{C-P} = 12 Hz), 21.4 (several peaks overlapped between 128 and 129 ppm); ^{31}P-NMR (160 MHz, $CDCl_3$) δ 29.3.

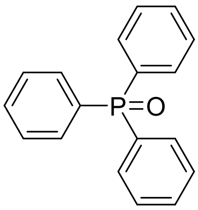
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[4]



2c

2c: 86% yield; white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.41-7.40 (m, 3H), 7.32-7.30 (m, 3H), 7.17-7.06 (m, 6H), 2.50 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 143.5 (d, J_{C-P} = 8 Hz), 132.9 (d, J_{C-P} = 12 Hz), 132.0 (d, J_{C-P} = 10 Hz), 131.8 (d, J_{C-P} = 2 Hz), 130.8 (d, J_{C-P} = 101 Hz), 125.4 (d, J_{C-P} = 12 Hz), 21.9 (d, J_{C-P} = 4 Hz); ^{31}P-NMR (160 MHz, $CDCl_3$) δ 37.0.

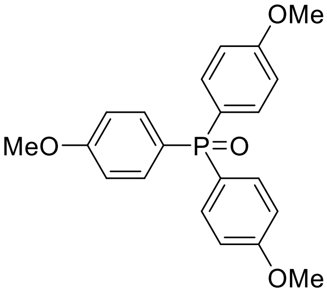
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[4]



2d

2d: 83% yield; white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.69-7.65 (m, 6H), 7.54-7.52 (m, 3H), 7.47-7.45 (m, 6H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 132.6 (d, J_{C-P} = 103 Hz), 132.1 (d, J_{C-P} = 10 Hz), 131.9, 128.5 (d, J_{C-P} = 12 Hz); ^{31}P-NMR (160 MHz, $CDCl_3$) δ 28.9.

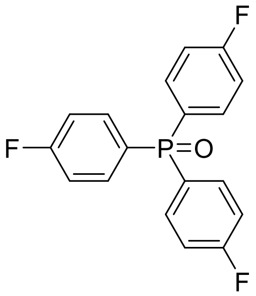
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[4]



2e

2e: 99% yield; white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, J = 8.8, 2.7 Hz, 6H), 6.93-6.91 (m, 6H), 3.80 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 162.2, 133.7 (d, J_{C-P} = 10 Hz), 124.5 (d, J_{C-P} = 109 Hz), 113.9 (d, J_{C-P} = 12 Hz), 55.2; ^{31}P-NMR (160 MHz, $CDCl_3$) δ 28.8.

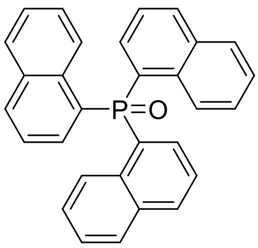
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[4]



2f

2f: 87% yield; white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.67-7.60 (m, 6H), 7.19-7.14 (m, 6H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 165.2 (dd, *J* = 253, 3 Hz), 134.4 (dd, *J* = 11, 9 Hz), 128.2 (dd, *J* = 107.5, 3 Hz), 116.1 (dd, *J* = 21, 13 Hz); ^{19}F-NMR (376 MHz, $CDCl_3$) δ –106.0; ^{31}P-NMR (160 MHz, $CDCl_3$) δ 26.7.

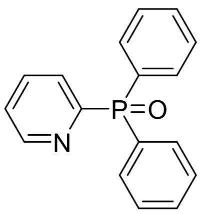
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[4]



2g

2g: 90% yield; white solid; ^{1}H-NMR (400 MHz, CD_2Cl_2) δ 8.89 (d, *J* = 8.6 Hz, 3H), 8.07 (d, *J* = 8.2 Hz, 3H), 7.98 (d, *J* = 8.2 Hz, 3H), 7.58-7.54 (m, 3H), 7.49-7.45 (m, 3H), 7.33-7.28 (m, 3H), 7.26-7.20 (m, 3H); ^{13}C-NMR (100 MHz, CD_2Cl_2) δ 134.8 (d, $J_{C\text{-}P}$ = 8.4 Hz), 156.4 (d, $J_{C\text{-}P}$ = 8.9 Hz), 134.0 (d, $J_{C\text{-}P}$ = 11.8 Hz), 133.6 (d, $J_{C\text{-}P}$ = 2.6 Hz), 129.5 (d, $J_{C\text{-}P}$ = 101.2 Hz), 129.3, 128.5 (d, $J_{C\text{-}P}$ = 4.7 Hz), 127.6, 126.9, 124.9 (d, $J_{C\text{-}P}$ = 14.4 Hz); ^{31}P-NMR (160 MHz, CD_2Cl_2) δ 39.5.

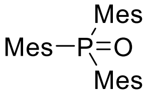
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[5]



2h

2h: 76% yield; white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.76 (d, *J* = 4.4 Hz, 1H), 8.31-8.28 (m, 1H), 7.90-7.81 (m, 5H), 7.52-7.48 (m, 2H), 7.45-7.41 (m, 4H), 7.38-7.34 (m, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 156.4 (d, $J_{C\text{-}P}$ = 131 Hz), 150.1 (d, $J_{C\text{-}P}$ = 19 Hz), 136.1 (d, $J_{C\text{-}P}$ = 9 Hz), 132.2 (d, $J_{C\text{-}P}$ = 103 Hz), 132.1 (d, $J_{C\text{-}P}$ = 9 Hz), 131.8 (d, $J_{C\text{-}P}$ = 3 Hz), 128.4 (d, $J_{C\text{-}P}$ = 7 Hz), 128.3 (d, $J_{C\text{-}P}$ = 12 Hz), 125.2 (d, $J_{C\text{-}P}$ = 3 Hz); ^{31}P-NMR (160 MHz, $CDCl_3$) δ 20.8.

^{1}H and ^{13}C NMR charts were consistent with previously reported data.[6]

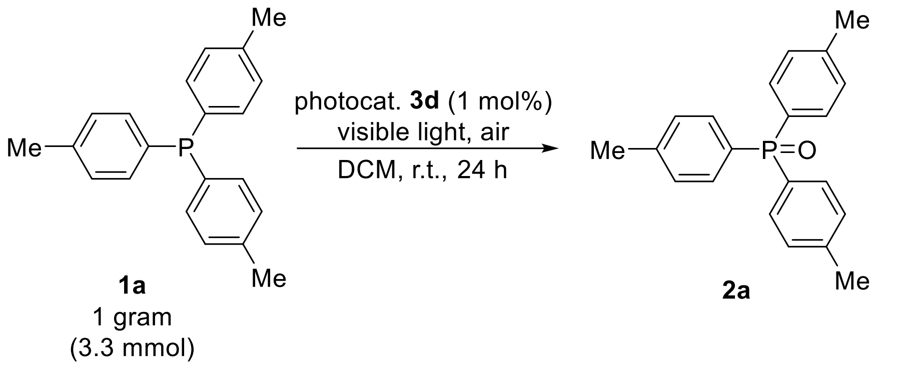


2i

2i: 54% yield; white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.82 (s, 6H), 2.53 (s, 9H), 2.27 (s, 9H), 1.85 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 140.6 (d, $J_{C\text{-}P}$ = 2 Hz), 132.6, 131.7, 131.1, 25.5, 21.0; ^{31}P-NMR (160 MHz, $CDCl_3$) δ 27.0.

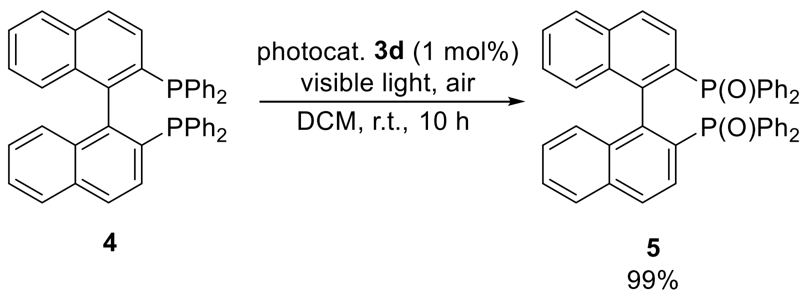
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[5]

Gram-Scale synthesis of 2a



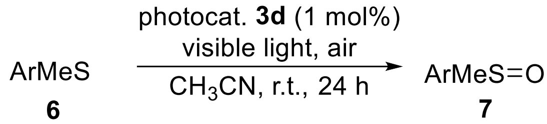
Tri(*p*-tolyl)phosphine **1a** (1 gram, 3.3 mmol), DBAB **3d** (18.3 mg, 0.033 mmol), and DCM (33 mL) were added to 100 mL round bottom flask with a stir bar. The mixture was irradiated by a white LED at room temperature under air atmosphere. After 24 h, the solvent was removed and the residue was purified by flash column chromatography on silica gel (Hexane/AcOEt = 1/1) to afford **2a** as a solid (942 mg, 89%)

Photooxidation of BINAP 4, thioanisoles 6, and triphenyl phosphite 8

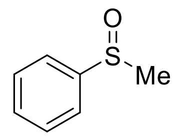


rac-BINAP **4** (125 mg, 0.2 mmol), DBAB **3d** (1.2 mg, 2 μmol), and DCM (4 mL) were added to a screw vial with a stir bar. The mixture was irradiated by a white LED at room temperature under air atmosphere. After 10 h, the solvent was removed and the residue was purified by flash column chromatography on silica gel (Hexane/AcOEt = 1/1 to 0/100) to afford BINAPO **5** as a solid (131 mg, 99%).

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.82-7.79 (m, 4H), 7.71-7.66 (m, 4H), 7.45-7.32 (m, 12H), 7.26-7.20 (m, 8H), 6.79 (d, J = 3.7 Hz, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 143.1, 143.0, 135.1, 134.0 (d, $J_{C\text{-}P}$ = 3.7 Hz), 133.6, 133.4 (d, $J_{C\text{-}P}$ = 11.6 Hz), 132.5 (d, $J_{C\text{-}P}$ = 10.3 Hz), 132.0 (d, $J_{C\text{-}P}$ = 9.0 Hz), 131.1 (d, $J_{C\text{-}P}$ = 2.5 Hz), 130.9 (d, $J_{C\text{-}P}$ = 2.8 Hz), 129.1 (d, $J_{C\text{-}P}$ = 102.6 Hz), 128.18, 127.9 (d, $J_{C\text{-}P}$ = 7.3 Hz), 127.8, 127.7, 127.3 (d, $J_{C\text{-}P}$ = 12.8 Hz), 123.1 (several peaks overlapped); ^{31}P-NMR (160 MHz, $CDCl_3$) δ 28.2. ^{1}H and ^{13}C NMR charts were consistent with previously reported data.[6]



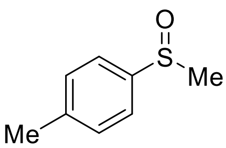
Thioanisole **6** (0.2 mmol), DBAB **3d** (1.2 mg, 2 µmol), and CH_3CN (2 mL) were added to a screw vial with a stir bar. The mixture was irradiated by a white LED at room temperature under air atmosphere. After 24 h, the solvent was removed and the residue was purified by flash column chromatography on silica gel (Hexane/AcOEt = 1/1 to 0/100) to afford sulfoxide **7**.



7a

7a: 95% yield; colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.65-7.62 (m, 2H), 7.54-7.48 (m, 3H), 2.71 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 145.7, 131.0, 129.3, 123.4, 43.9.

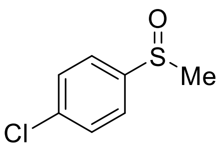
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[7]



7b

7b: 76% yield; colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.52 (d, J = 8 Hz, 2H), 7.31 (d, J = 8 Hz, 2H), 2.69 (s, 3H), 2.40 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 142.4, 141.6, 130.0, 123.6, 43.9, 21.4.

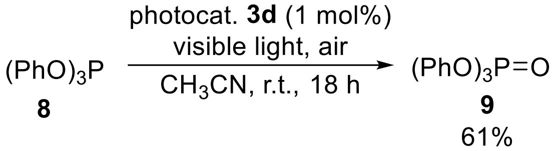
^{1}H and ^{13}C NMR charts were consistent with previously reported data.[7]



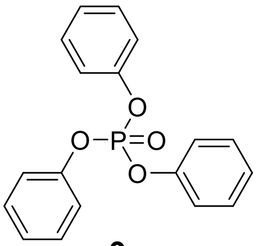
7c

7c: 74% yield; colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 2.72 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 143.8, 137.4, 129.7, 125.0, 43.8.

^{1}H and ^{13}C NMR charts were consistent with previously reported data.[7]



Triphenyl phosphite **8** (52 μL, 0.2 mmol), DBAB **3d** (1.2 mg, 2 µmol), and CH_3CN (2 mL) were added to a screw vial with a stir bar. The mixture was irradiated by a white LED at room temperature under air atmosphere. After 18 h, the solvent was removed and the residue was purified by flash column chromatography on silica gel (Hexane/AcOEt = 5/1) to afford triphenyl phosphate **9** (40 mg, 61%).



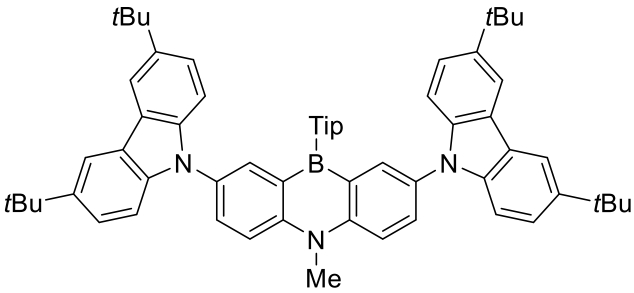
9

9: 61% yield; white solid; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.37-7.33 (m, 6H), 7.25-7.19 (m, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 150.5 (d, J_{C-P} = 7 Hz), 129.8, 125.6, 120.1 (d, J_{C-P} = 5 Hz); ^{31}P-NMR (160 MHz, $CDCl_3$) δ -17.7.

^{1}H and ^{13}C NMR charts were consistent with previously reported data.[8]

Preparation and characterization of 3e and 3f

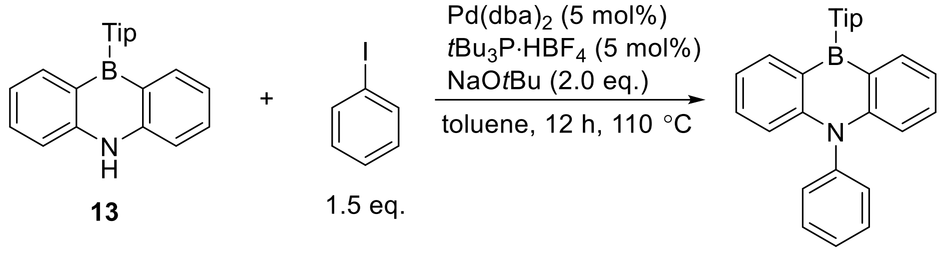
DBAB **3e** was obtained as a yellow solid according to the previously reported procedure using DBAB **3d**.[9]



3e

^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.15-8.14 (m, 6H), 7.96 (d, J = 9.2 Hz, 2H), 7.89 (d, J = 9.2 Hz, 2H), 7.41 (dd, J = 8.8, 1.6 Hz, 4H), 7.19 (d, J = 8.8 Hz, 4H), 6.92 (s, 2H), 4.31 (s, 3H), 2.84-2.77 (m, 1H), 2.79-2.77 (m, 2H), 1.47 (s, 36H), 1.21 (d, J = 7.2 Hz, 6H), 1.05 (d, J = 6.8 Hz, 12H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 149.9, 148.1, 145.0, 142.5, 140.0, 136.2, 132.9, 129.8, 123.4, 123.0, 120.0, 116.6, 116.2, 109.0, 36.2, 35.2, 34.7, 34.2, 32.0, 24.4, 24.0 (Two ^{13}C NMR signals attributable to the aromatic carbon atoms ipso to the B atom could not be observed, because of the substantial signal broadening due to the quadrupolar boron nuclei); IR (KBr) 3046, 2959, 1630, 1555, 1476, 1229, 876 cm^{-1}; HRMS (APCI): calcd for $C_{68}H_{81}BN_3$: m/z 950.6518 ([M+H]+), found: m/z 950.6522.

DBAB **3f**



DBAB **13** (76.3 mg, 0.2 mmol), iodobenzene (33 µL, 0.3 mmol), sodium *tert*-butoxide (38.4 mg, 0.4 mmol), $Pd(dba)_2$ (5.8 mg, 0.01 mmol), and $t$$Bu_3P{\cdot}HBF_4$ (2.9 mg, 0.01 mmol) in dry toluene (4 mL) were stirred under Ar atmosphere at 110 °C for 12 h. The reaction mixture was cooled down to room temperature and extracted with water and dichloromethane. The organic layer was dried over Na_2SO_4, removed under reduced pressure, and then purified by column chromatography (Hexane/DCM =9/1) to afford DBAB **3f** (80.2 mg, 0.175 mmol, 88%) as a white solid.

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 7.6, 1.6 Hz, 2H), 7.75-7.71 (m, 2H), 7.66-7.64 (m, 1H), 7.50-7.45 (m, 4H), 7.12-7.08 (m, 4H), 6.82 (d, *J* = 8.8 Hz, 2H), 3.06-2.99 (m, 1H), 2.53-2.46 (m, 2H), 1.34 (d, *J* = 6.8 Hz, 6H), 1.04 (d, *J* = 6.8 Hz, 12H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 150.5, 147.8, 146.3, 141.8, 137.6, 132.5, 130.8, 130.5, 128.8, 119.7, 119.4, 116.7, 35.1, 34.3, 24.4, 24.2 (Two ^{13}C NMR signals attributable to the aromatic carbon atoms ipso to the B atom could not be observed, because of the substantial signal broadening due to the quadrupolar boron nuclei); IR (KBr) 3063, 2953, 1597, 1568, 1468, 1236, 874 cm^{-1}; HRMS (APCI): calcd for C33H37BN: m/z 458.3014 ([M+H]+), found: m/z 458.3018

Cyclic voltammograms and UV-vis spectra of 3a and 3d

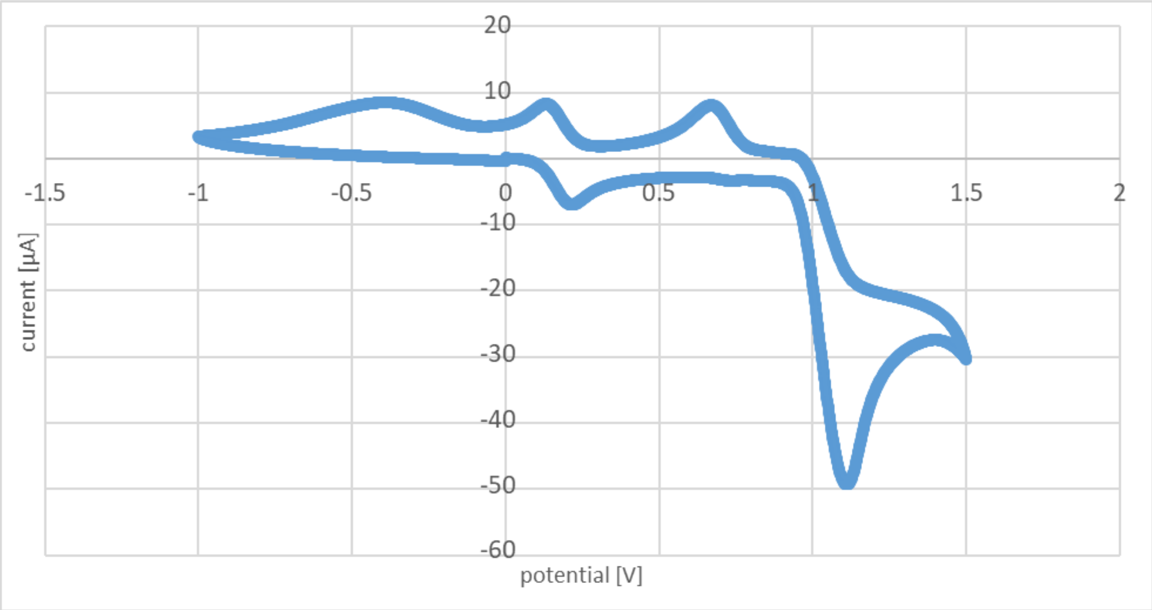


Fig. S1. Cyclic voltammogram for **3a** (1 mM in DCM). Conditions: a glassy carbon working electrode, a $Ag/AgNO_3$ reference electrode, and a Pt wire counter electrode, Bu_4NPF_6 (0.1 M in DCM), 100 mV/s scan rate.

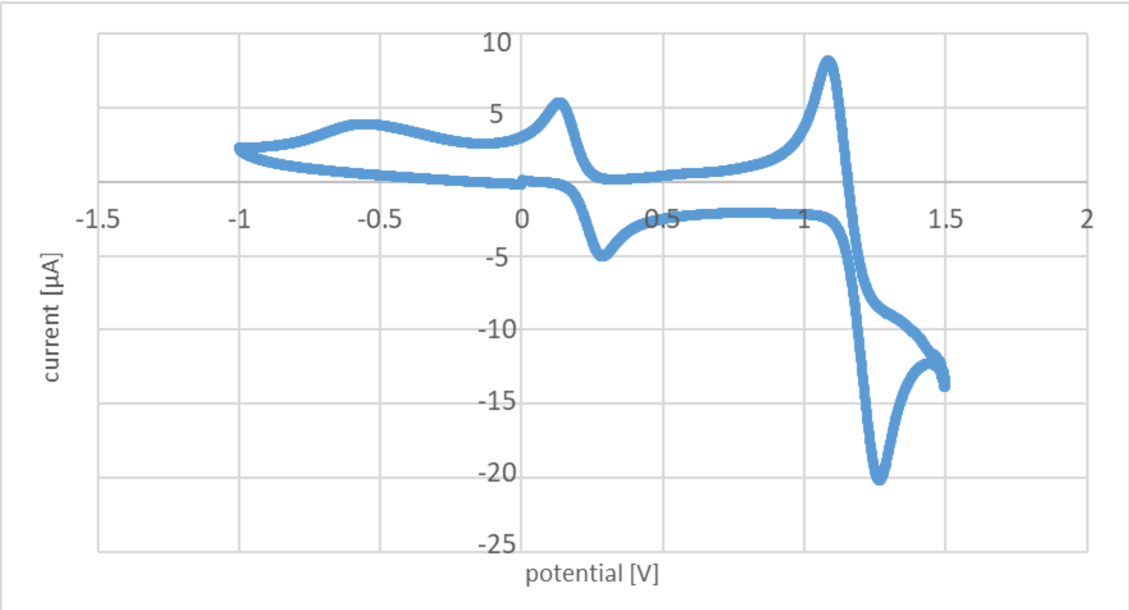


Fig. S2. Cyclic voltammogram for **3d** (1 mM in DCM). Conditions: a glassy carbon working electrode, a $Ag/AgNO_3$ reference electrode, and a Pt wire counter electrode, Bu_4NPF_6 (0.1 M in DCM), 100 mV/s scan rate.

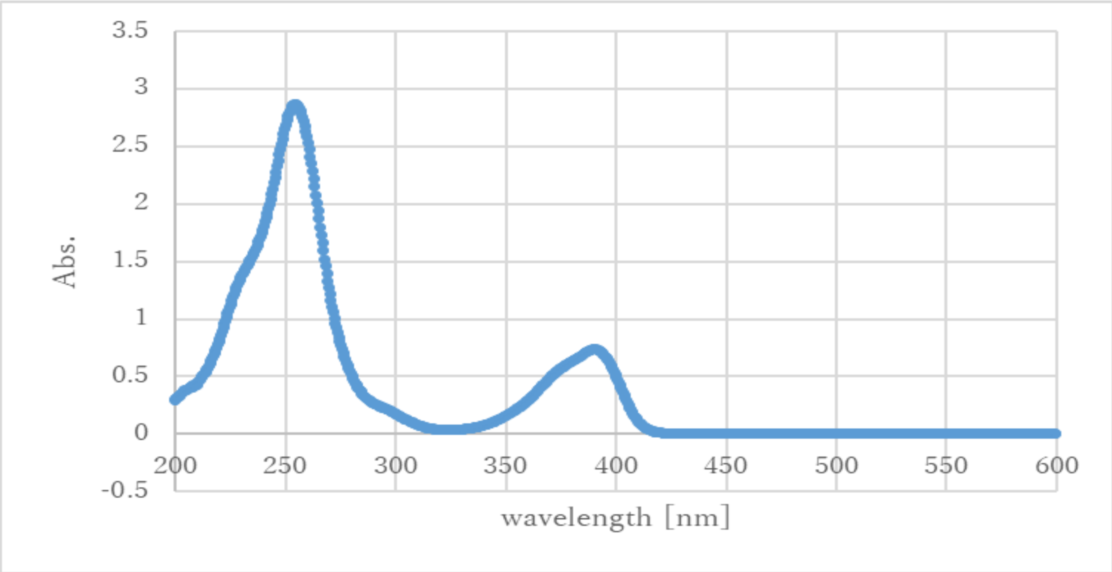


Fig. S3. UV-vis spectrum of **3a** (0.1 mM in DCM).

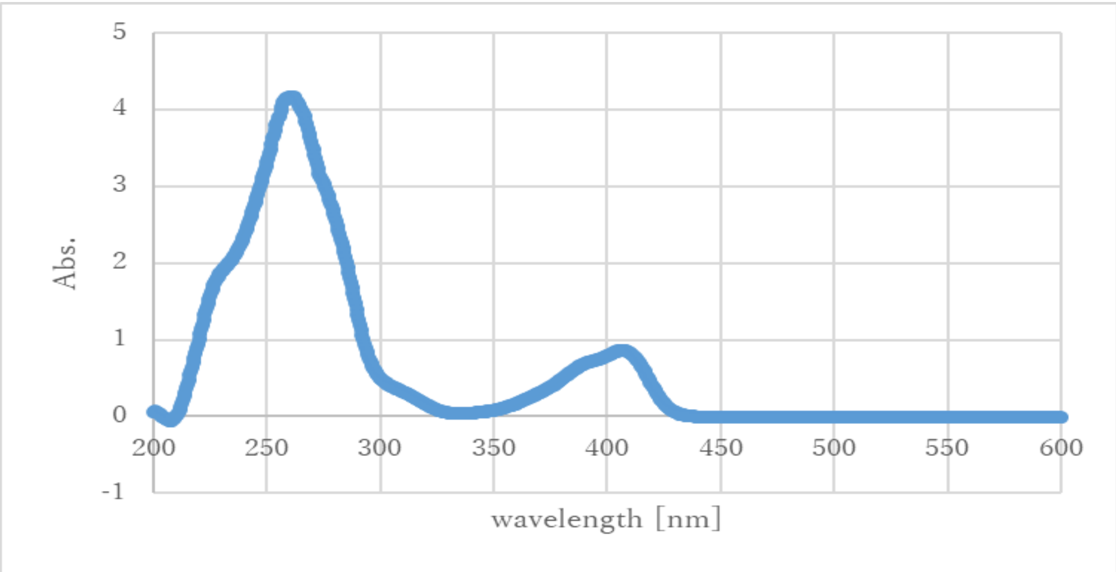
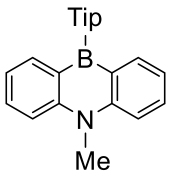


Fig. S4. UV-vis spectrum of **3d** (0.1 mM in DCM).

Details of the DFT calculations

DFT calculations were performed using Gaussian 16 (revision C.01).[10] Geometry optimizations were carried out at the CAM-B3LYP/6-311G(d) level of theory, and the frequency calculations confirmed that all the optimized geometries correspond to the equilibrium structures. Computational time was provided by the SuperComputer Laboratory, Institute for Chemical Research, Kyoto University and by Research Center for Computational Science, Okazaki, Japan.

Dibenzoazaborine **3a**



3a

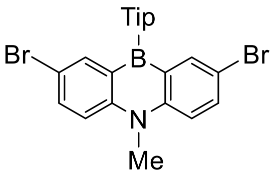
C	-1.78461	-3.71755	0.180037
C	-3.17462	-3.62921	0.108031
C	-3.80508	-2.41204	-0.03067
C	-3.05491	-1.22147	-0.10376
N	-3.70143	0.000013	-0.27575
C	-3.0549	1.22149	-0.10375
C	-3.80506	2.412065	-0.03064
C	-3.17459	3.629229	0.108071
C	-1.78457	3.717551	0.18008
C	-1.0497	2.555158	0.136736
B	-0.82298	-3E-06	0.017447
C	-1.64763	1.288363	0.006957
C	-1.64764	-1.28836	0.006941
C	-1.04973	-2.55516	0.136704
H	-1.29904	-4.6811	0.282181
H	-4.88556	-2.39297	-0.04053
H	-4.88554	2.393002	-0.0405
H	-3.7787	4.528253	0.171603
H	-1.29899	4.681092	0.282236
H	0.031803	-2.59706	0.207826
H	-3.77875	-4.52823	0.171555

H	0.031828	2.597038	0.207861
C	-5.10033	0.000022	-0.67801
H	-5.3047	-0.87218	-1.29257
H	-5.78542	0.000019	0.175457
H	-5.30469	0.872236	-1.29256
C	0.756487	-0.00001	0.079137
C	1.431393	-2.9E-05	1.309326
C	1.512659	0.000003	-1.1061
C	2.824261	-3.6E-05	1.333683
C	2.901285	-2E-06	-1.04376
C	3.579986	-2.2E-05	0.170143
H	3.341445	-5.2E-05	2.289163
H	3.471113	0.000009	-1.96815
C	0.828007	0.00002	-2.46587
C	1.151405	-1.26273	-3.26881
C	1.151427	1.262771	-3.2688
H	-0.25325	0.000029	-2.29528
H	0.878139	-2.16352	-2.71577
H	0.605829	-1.27059	-4.21611
H	2.217206	-1.3268	-3.50196
H	0.878175	2.163567	-2.71574

H	2.217229	1.326826	-3.50194
H	0.605852	1.270659	-4.2161
C	0.6663	-3.9E-05	2.625633
C	0.943038	1.261545	3.448185
C	0.943069	-1.26161	3.448192
H	-0.40253	-5.3E-05	2.391275
H	0.701753	2.163974	2.883244
H	0.343183	1.267392	4.362029
H	1.993481	1.324822	3.743026
H	0.701819	-2.16405	2.883251
H	1.99351	-1.32486	3.743047
H	0.343202	-1.26747	4.362028

C	5.095644	-2.2E-05	0.22867
C	5.690722	1.261417	-0.40304
C	5.690741	-1.26137	-0.4032
H	5.375341	-0.00009	1.287787
H	5.292239	2.164218	0.06401
H	6.778425	1.275749	-0.29461
H	5.465706	1.315532	-1.47115
H	5.292254	-2.16424	0.063708
H	5.465751	-1.31534	-1.47133
H	6.778442	-1.27571	-0.29475

Dibenzoazaborine **3d**



3d

C	3.699633	-1.56455	0.07467
C	3.62948	-2.95266	-0.01486
C	2.411367	-3.57631	-0.16293
C	1.219478	-2.82774	-0.22637
N	-2.2E-05	-3.4731	-0.40599
C	-1.21951	-2.82773	-0.22637
C	-2.41141	-3.57629	-0.16292
C	-3.62952	-2.95262	-0.01486
C	-3.69966	-1.5645	0.074669
C	-2.54832	-0.81828	0.042628
B	-6E-06	-0.59237	-0.07584
C	-1.28663	-1.42342	-0.09657
C	1.286609	-1.42343	-0.09657
C	2.548303	-0.8183	0.042631
H	2.398128	-4.65638	-0.18745
H	-2.39819	-4.65635	-0.18744

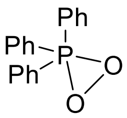
H	-4.53307	-3.54694	0.042569
H	2.594838	0.260423	0.128152
H	4.533023	-3.54699	0.042563
H	-2.59484	0.260452	0.128147
C	-3.1E-05	-4.86882	-0.82286
H	0.871468	-5.06681	-1.44029
H	-3.7E-05	-5.56111	0.024322
H	-0.87153	-5.0668	-1.44029
C	0.000005	0.983245	0.00445
C	0.00001	1.642279	1.243281
C	0.000013	1.751888	-1.17281
C	0.000022	3.034518	1.283307
C	0.000023	3.139315	-1.09372
C	0.000028	3.803315	0.128351
H	0.000026	3.540627	2.244455
H	0.000028	3.720195	-2.01097

C	0.000008	1.082452	-2.54003	H	-1.32149	2.174185	3.686676
C	1.262633	1.41493	-3.33952	H	2.166044	0.899406	2.809467
C	-1.26262	1.414933	-3.33951	H	1.321475	2.17419	3.686687
H	0.000007	-0.00136	-2.38195	H	1.268348	0.515323	4.281155
H	2.165051	1.140046	-2.78992	C	0.000045	5.318064	0.204268
H	1.271327	0.87834	-4.29181	C	-1.26163	5.919594	-0.4208
H	1.324061	2.48278	-3.56301	C	1.261745	5.919564	-0.42078
H	-2.16504	1.140073	-2.7899	H	0.000038	5.585545	1.266442
H	-1.32404	2.48278	-3.56303	H	-2.16464	5.515361	0.04075
H	-1.27133	0.878325	-4.29179	H	-1.27616	7.005747	-0.29892
C	0	0.861301	2.550099	H	-1.3151	5.708098	-1.4917
C	-1.26147	1.128249	3.37617	H	2.16474	5.515337	0.040812
C	1.261454	1.12825	3.376192	H	1.315245	5.708031	-1.49167
H	0.000003	-0.20533	2.303142	H	1.276278	7.00572	-0.29894
H	-2.16605	0.899419	2.809423	Br	-5.39583	-0.72151	0.263268
H	-1.26839	0.51531	4.281124	Br	5.395813	-0.72157	0.263272

Ph_3P

P	-3.8E-05	-8.7E-05	-1.22894	C	0.125899	4.009882	-0.45892
C	-1.59201	-0.45451	-0.41787	H	-0.73142	2.675477	-1.89829
C	-2.32798	-1.48675	-1.00283	C	0.922622	4.128914	0.671899
C	-2.10761	0.173623	0.714437	H	2.091412	3.077729	2.133894
C	-3.53552	-1.8964	-0.45852	H	-0.29402	4.894537	-0.92505
H	-1.95079	-1.97259	-1.89728	H	1.1266	5.106767	1.094164
C	-3.32315	-0.22782	1.253058	C	1.189612	-1.15159	-0.41798
H	-1.55969	0.985047	1.178671	C	2.451785	-1.27204	-1.00255
C	-4.03747	-1.26512	0.671636	C	0.903375	-1.91262	0.714038
H	-4.09145	-2.70279	-0.92428	C	3.410576	-2.1126	-0.45811
H	-3.71225	0.273844	2.132562	H	2.683982	-0.70206	-1.89672
H	-4.98644	-1.57717	1.093769	C	1.859057	-2.76428	1.25272
C	0.402473	1.605809	-0.41784	H	-0.07351	-1.84433	1.177981
C	1.203326	1.738211	0.715103	C	3.114772	-2.8635	0.67165
C	-0.12282	2.759269	-1.00335	H	4.387114	-2.19019	-0.9235
C	1.463132	2.991611	1.253874	H	1.619168	-3.35248	2.131958
H	1.631673	0.857963	1.17971	H	3.859681	-3.52907	1.093837

Ph_3PO_2



P	-0.02057	-0.12732	0.885023	H	1.573713	2.148603	1.662766
C	1.462671	-0.89464	0.150804	C	0.345577	4.234989	-0.69999
C	1.94048	-2.10925	0.648392	H	-1.14894	3.712863	-2.14915
C	2.096287	-0.32081	-0.95313	H	1.798759	4.463487	0.866409
C	3.026812	-2.73184	0.053938	H	0.442881	5.256902	-1.04979
H	1.467759	-2.54531	1.517234	C	-1.53729	-0.74271	0.099573
C	3.178142	-0.95147	-1.55003	C	-2.74555	-0.58655	0.776144
H	1.752439	0.625857	-1.34856	C	-1.51961	-1.35089	-1.15063
C	3.645391	-2.15672	-1.04723	C	-3.92429	-1.02814	0.19836
H	3.392814	-3.66971	0.456121	H	-2.75648	-0.1323	1.760239
H	3.66069	-0.49348	-2.40605	C	-2.70454	-1.79589	-1.72416
H	4.495226	-2.64578	-1.51069	H	-0.58308	-1.48921	-1.67919
C	0.091839	1.5997	0.202269	C	-3.90625	-1.63194	-1.05318
C	-0.67278	2.06117	-0.86614	H	-4.86145	-0.90679	0.72986
C	0.98021	2.484064	0.819499	H	-2.68392	-2.27505	-2.69659
C	-0.54437	3.369579	-1.31675	H	-4.83031	-1.98019	-1.50109
H	-1.38246	1.402584	-1.35227	O	-0.13088	0.319273	2.429077
C	1.10667	3.78982	0.373228	O	-0.11231	-1.19348	2.278372

Ph_3PO

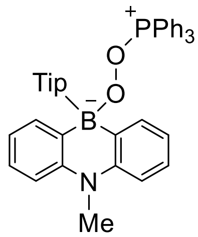
P	0.000178	-0.00135	0.92163	H	-5.04725	-1.67933	-1.09066
C	-1.58122	-0.57376	0.221759	C	1.286328	-1.08232	0.22002
C	-2.72582	-0.34586	0.984224	C	1.900589	-0.85293	-1.00866
C	-1.69322	-1.21819	-1.00835	C	1.662555	-2.1886	0.980301
C	-3.96777	-0.74083	0.510911	C	2.865775	-1.73151	-1.4808
H	-2.63032	0.124279	1.956296	H	1.642873	0.023724	-1.59239
C	-2.93818	-1.61096	-1.47986	C	2.627444	-3.06406	0.506168
H	-0.80679	-1.43414	-1.59431	H	1.206658	-2.34388	1.951408
C	-4.07546	-1.36886	-0.72279	C	3.226538	-2.83867	-0.72588
H	-4.85416	-0.56381	1.109708	H	3.343758	-1.54483	-2.43604
H	-3.0184	-2.11559	-2.43628	H	2.917969	-3.92099	1.103566

H	3.983865	-3.52215	-1.09393	H	-0.84951	1.416772	-1.58694
C	0.294231	1.653874	0.222182	C	0.849295	4.212213	-0.72188
C	1.069103	2.529306	0.981066	H	1.94888	4.47938	1.103865
C	-0.21529	2.07506	-1.00394	H	-0.33922	3.674421	-2.42772
C	1.347356	3.802254	0.507826	H	1.064772	5.209618	-1.08906
H	1.434353	2.209391	1.950214	O	0.002472	-0.00416	2.412894
C	0.064437	3.350613	-1.47485				

O_2

O	0	0	0.598303	O	0	0	-0.5983

Complex of dibenzoazaborine **3a** and Ph_3PO_2

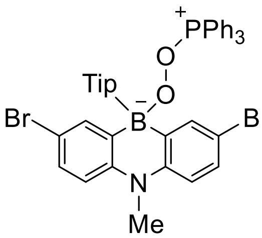


N	0.674211	-3.11507	-0.06524	C	-5.20617	0.912081	-0.09092
C	-0.73189	-1.60746	-1.38622	H	-1.8793	-0.40364	-2.71492
C	-0.58006	-1.46741	1.234851	H	-1.63753	-0.16362	2.542331
C	0.070854	-2.75884	-1.28867	H	0.817118	-4.49664	-2.34784
C	0.229751	-2.61926	1.17024	H	1.158948	-4.20063	2.328294
C	-2.47677	0.012666	-0.04709	H	1.393631	-5.12514	0.024382
C	-1.25619	-1.28988	-2.6359	H	2.438066	-3.88333	0.736258
C	-0.996	-1.03855	2.492261	H	2.302861	-4.00843	-1.00544
C	0.271422	-3.5647	-2.41921	H	-1.44926	-1.77339	-4.72695
C	0.587865	-3.28212	2.356147	H	-0.98031	-1.31327	4.630853
C	-3.57141	-0.8955	-0.05408	H	-0.098	-3.85274	-4.50563
C	-2.81608	1.386539	0.004448	H	0.449036	-3.34966	4.488237
C	1.74208	-4.08889	-0.07602	H	-5.6948	-1.15672	-0.09503
C	-1.02514	-2.05775	-3.76959	H	-4.36205	2.865222	-0.00867
C	-0.62962	-1.67747	3.670592	O	0.109322	0.498548	-0.26498
C	-0.26569	-3.20942	-3.64743	O	1.3949	-0.20251	-0.43443
C	0.167951	-2.80809	3.590279	P	2.591636	0.77049	-0.07327
C	-4.88424	-0.4339	-0.08268	C	2.756114	2.093986	-1.27858
C	-4.14863	1.800911	-0.03281	C	4.005349	-0.32688	-0.21184

C	2.455878	1.426861	1.585039
C	1.630599	2.560366	-1.95738
C	4.014317	2.641064	-1.53871
C	5.035076	-0.2979	0.725339
C	4.059922	-1.20695	-1.29504
C	2.071821	0.559483	2.609444
C	2.733811	2.766086	1.856491
C	1.771289	3.581001	-2.88608
H	0.663756	2.11626	-1.76045
C	4.140268	3.665355	-2.46251
H	4.896626	2.26149	-1.03516
C	6.125289	-1.1427	0.573228
H	4.982447	0.369232	1.577685
C	5.149279	-2.05019	-1.43303
H	3.245983	-1.24614	-2.00949
C	1.979569	1.039435	3.90504
H	1.812464	-0.47143	2.397853
C	2.644367	3.232645	3.158621
H	3.005029	3.444851	1.056787
C	3.018642	4.135032	-3.1344
H	0.897471	3.940524	-3.41631
H	5.11634	4.089861	-2.66645
C	6.18178	-2.01517	-0.50354
H	6.926288	-1.12375	1.302833
H	5.190202	-2.73997	-2.2677
C	2.269948	2.36956	4.179423
H	1.659076	0.370084	4.693595
H	2.854999	4.273705	3.373266
H	3.120835	4.932739	-3.86149
H	7.032564	-2.6774	-0.61729
H	2.190873	2.739835	5.195402

C	-1.80331	2.523536	0.126264
C	-2.02551	3.361074	1.391226
C	-1.80125	3.417983	-1.11824
H	-0.81371	2.092862	0.222984
H	-2.01277	2.732099	2.283839
H	-1.23625	4.111783	1.498825
H	-2.98051	3.891553	1.376804
H	-1.6343	2.831308	-2.02516
H	-2.75471	3.937072	-1.24335
H	-1.01962	4.181925	-1.0534
C	-3.42386	-2.41614	0.012389
C	-4.04607	-3.12159	-1.1964
C	-3.99839	-2.97179	1.320491
H	-2.36926	-2.66771	0.008723
H	-3.6112	-2.76156	-2.1295
H	-3.86903	-4.19941	-1.13936
H	-5.12764	-2.97097	-1.24704
H	-3.5213	-2.51047	2.186693
H	-5.07513	-2.7991	1.398
H	-3.83232	-4.05125	1.382042
B	-0.96774	-0.662	-0.10381
C	-6.64823	1.376923	-0.14103
C	-6.94195	2.18901	-1.40543
C	-7.04205	2.160776	1.11399
H	-7.27331	0.477709	-0.17585
H	-6.69302	1.622317	-2.30479
H	-7.99916	2.464101	-1.45871
H	-6.35871	3.113312	-1.4264
H	-6.86241	1.574836	2.017528
H	-6.46568	3.085482	1.201078
H	-8.10108	2.432989	1.090332

Complex of dibenzoazaborine **3d** and Ph_3PO_2



N	-0.68459	-0.34674	-3.01564
C	0.726167	-1.39596	-1.31452
C	0.286765	1.192772	-1.38541
C	0.007523	-1.46814	-2.52095
C	-0.41554	0.959483	-2.58352
C	2.204569	0.237297	0.302296
C	1.350464	-2.55052	-0.85366
C	0.518376	2.511587	-1.0062
C	-0.01474	-2.66909	-3.24346
C	-0.84367	2.049688	-3.35724
C	3.350239	0.294798	-0.53824
C	2.443149	0.415859	1.687104
C	-1.67944	-0.5447	-4.04686
C	1.278791	-3.74383	-1.55182
C	0.056485	3.577161	-1.76053
C	0.609711	-3.80767	-2.75839
C	-0.6202	3.353817	-2.94445
C	4.624534	0.449362	-0.00047
C	3.741409	0.561056	2.178305
C	4.855058	0.568392	1.358751
H	1.910246	-2.50503	0.073704
H	1.070749	2.699548	-0.09244
H	-0.49111	-2.72919	-4.21302
H	-1.32663	1.90017	-4.31347
H	-1.27326	-0.48778	-5.06468
H	-2.46529	0.202864	-3.9495
H	-2.14845	-1.51902	-3.92154
H	0.583651	-4.72728	-3.32984
H	-0.95431	4.181894	-3.5574

H	5.477576	0.481891	-0.67168
H	3.880535	0.678461	3.248465
O	-0.36177	-0.22998	0.641435
O	-1.59401	-0.53177	-0.11168
P	-2.84501	-0.31311	0.84279
C	-2.92318	-1.56433	2.128697
C	-4.21862	-0.54974	-0.28692
C	-2.85438	1.33431	1.536546
C	-1.74919	-2.13504	2.620622
C	-4.16547	-1.96518	2.625382
C	-5.26826	0.363228	-0.34916
C	-4.21711	-1.681	-1.10678
C	-2.50354	2.401114	0.706762
C	-3.19409	1.555497	2.870215
C	-1.82681	-3.09981	3.61381
H	-0.79321	-1.82806	2.21766
C	-4.22869	-2.92279	3.624064
H	-5.08198	-1.54473	2.226303
C	-6.31978	0.140944	-1.2271
H	-5.26248	1.24862	0.275242
C	-5.26768	-1.88968	-1.98341
H	-3.39241	-2.38326	-1.06927
C	-2.49839	3.688038	1.217456
H	-2.19957	2.226796	-0.31852
C	-3.19602	2.849403	3.368206
H	-3.44027	0.724979	3.521111
C	-3.05972	-3.48862	4.117305
H	-0.91568	-3.54842	3.991104
H	-5.19179	-3.23611	4.009642

C	-6.31875	-0.98184	-2.04102
H	-7.13656	0.851162	-1.27817
H	-5.266	-2.763	-2.62481
C	-2.84821	3.910425	2.543692
H	-2.19557	4.512212	0.583085
H	-3.45454	3.02627	4.40554
H	-3.11242	-4.2434	4.893724
H	-7.13995	-1.15082	-2.72825
H	-2.83534	4.919138	2.94066
C	1.351972	0.486972	2.753911
C	1.374075	1.818232	3.514413
C	1.434839	-0.69232	3.729317
H	0.387209	0.439178	2.263474
H	1.301928	2.664265	2.827708
H	0.53001	1.877471	4.208574
H	2.28738	1.947934	4.099663
H	1.422232	-1.64726	3.197985
H	2.355595	-0.66589	4.317192
H	0.596816	-0.68051	4.433552
C	3.297878	0.237641	-2.06534
C	4.092894	-0.94015	-2.63712

C	3.762491	1.559837	-2.6864
H	2.269122	0.097426	-2.3783
H	3.744298	-1.88952	-2.22845
H	3.981376	-0.98232	-3.72428
H	5.161026	-0.85567	-2.42218
H	3.169156	2.398842	-2.31886
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B	0.759869	-0.03355	-0.45162
C	6.259627	0.716862	1.909149
C	6.637712	-0.449	2.826856
C	6.457152	2.058264	2.620579
H	6.942734	0.69564	1.052822
H	6.527866	-1.40674	2.314514
H	7.67403	-0.36134	3.164914
H	6.00184	-0.47572	3.715592
H	6.21677	2.894463	1.961131
H	5.815202	2.138379	3.501631
H	7.491829	2.175547	2.954672
Br	0.360868	5.373296	-1.17193
Br	2.129929	-5.30983	-0.85946

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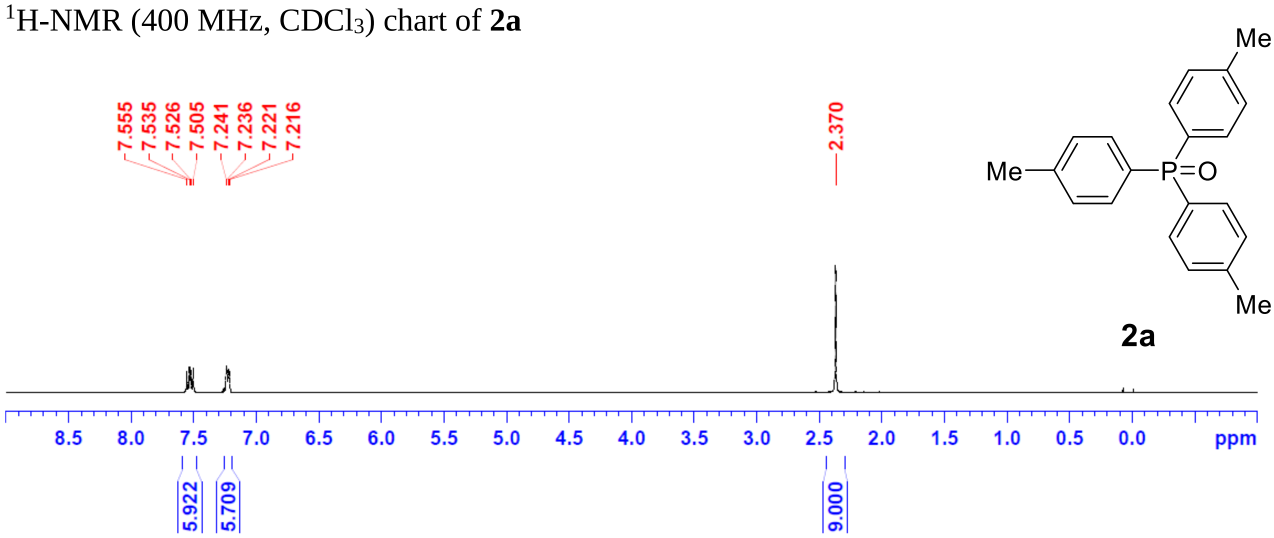
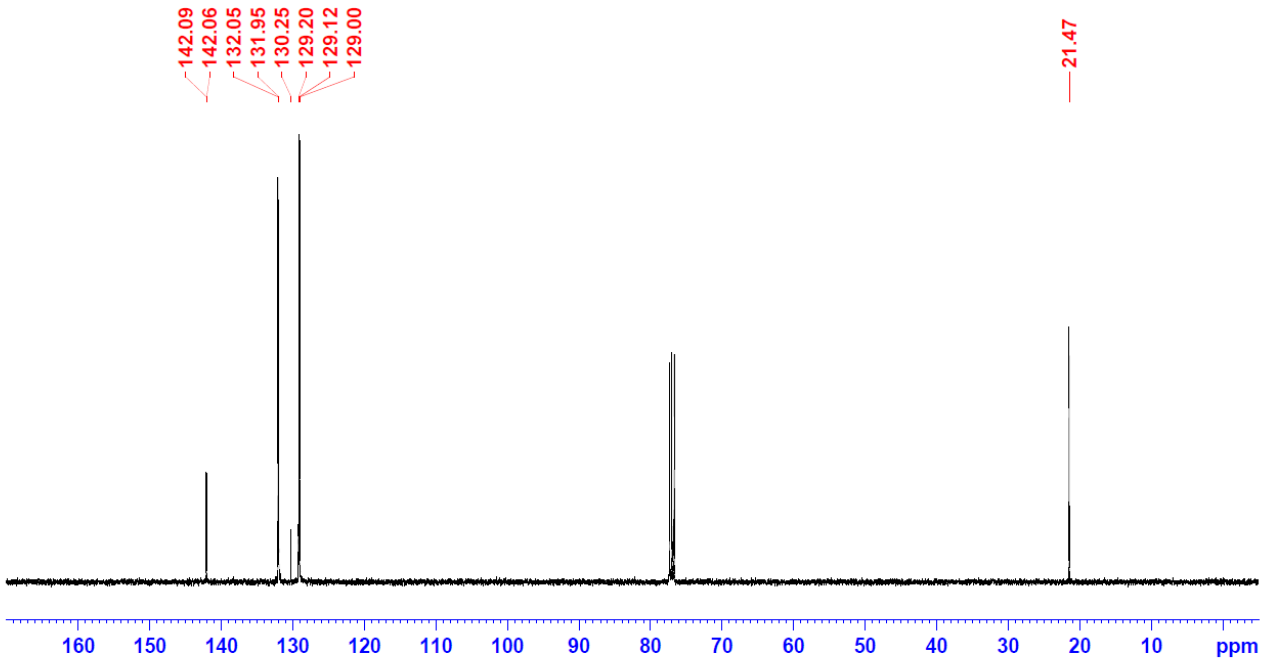
[1]H-NMR (400 MHz, $CDCl_3$) chart of **2a**

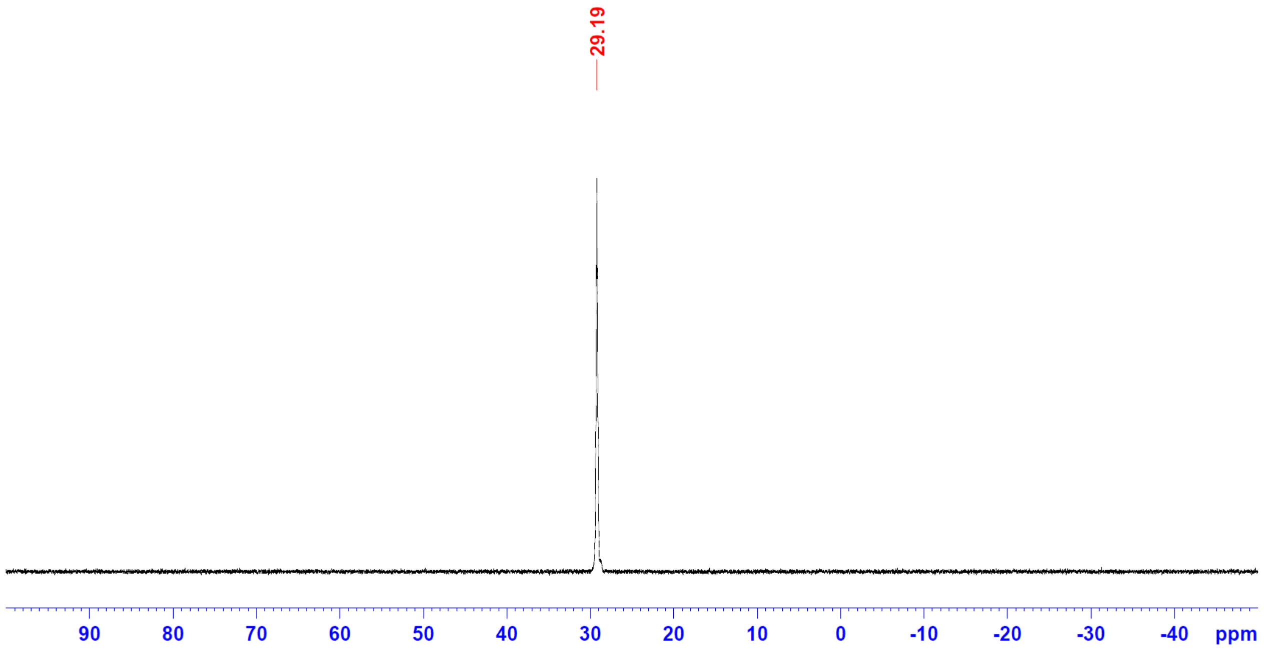


2a

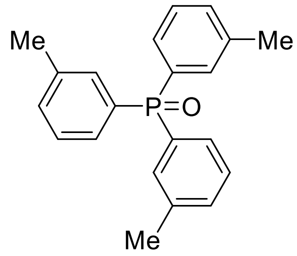
[13]C-NMR (100 MHz, $CDCl_3$) chart of **2a**



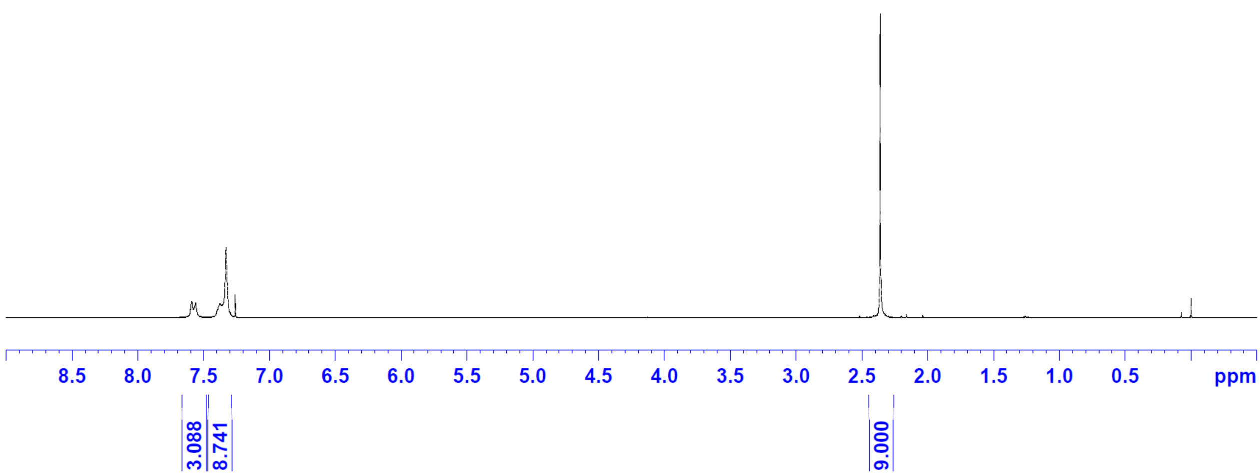
^{31}P-NMR (160 MHz, $CDCl_3$) chart of **2a**



[1]H-NMR (400 MHz, $CDCl_3$) chart of **2b**



2b



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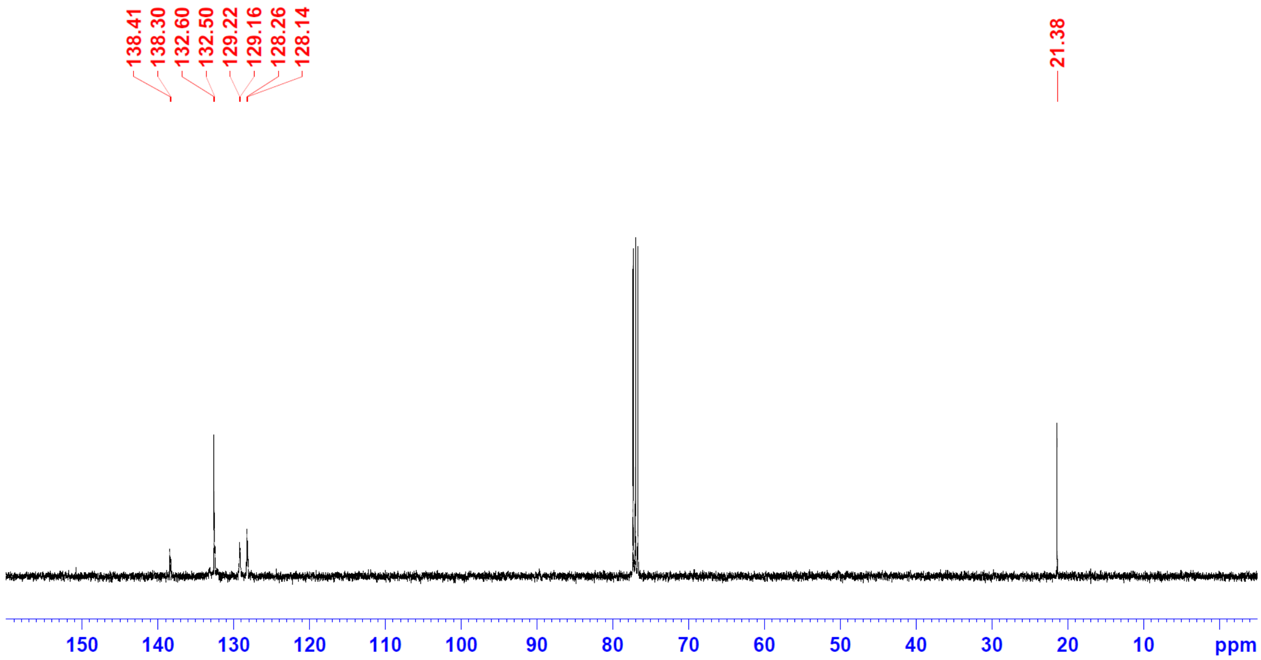

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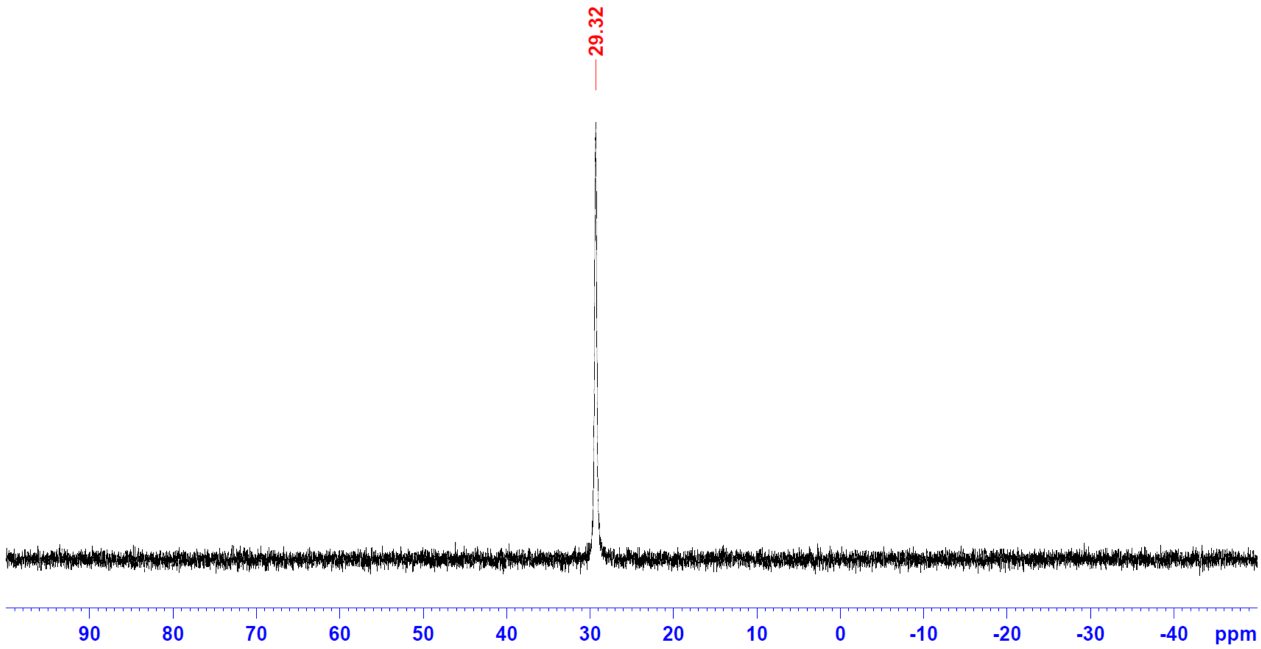
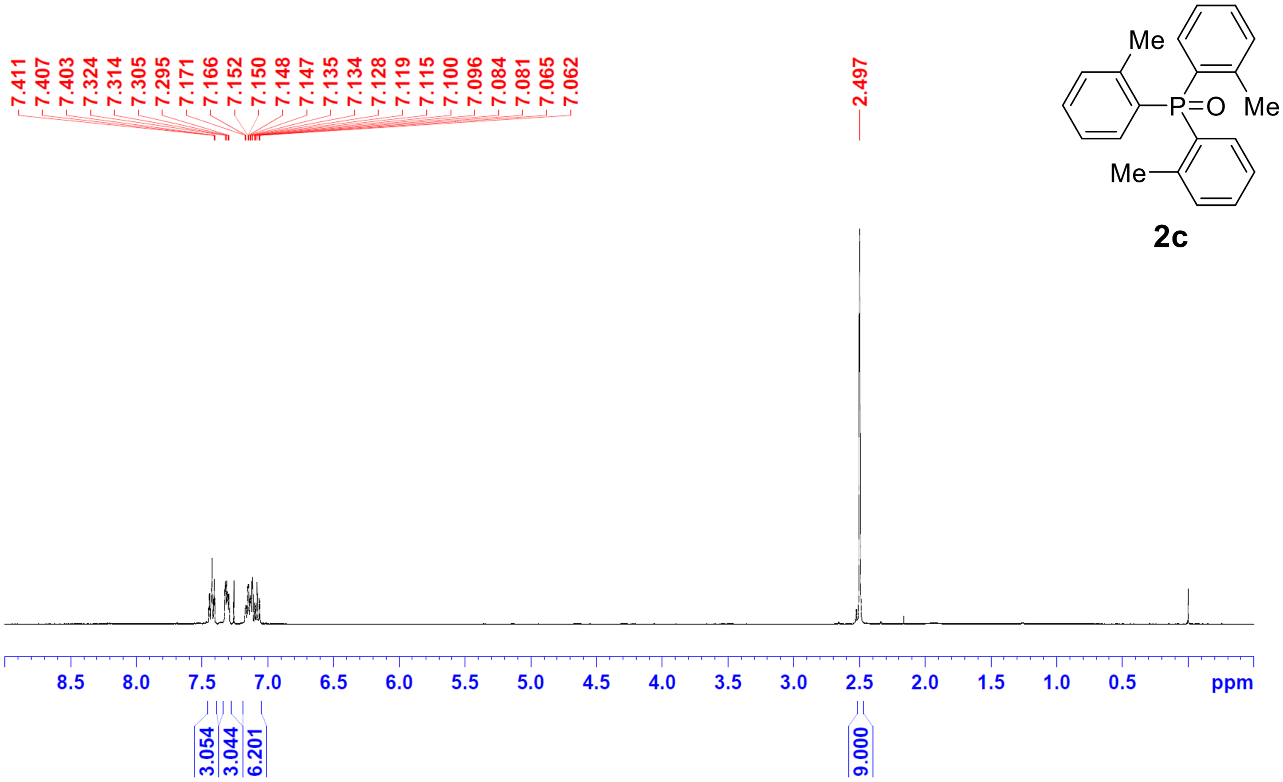


[1]H-NMR (400 MHz, $CDCl_3$) chart of **2c**



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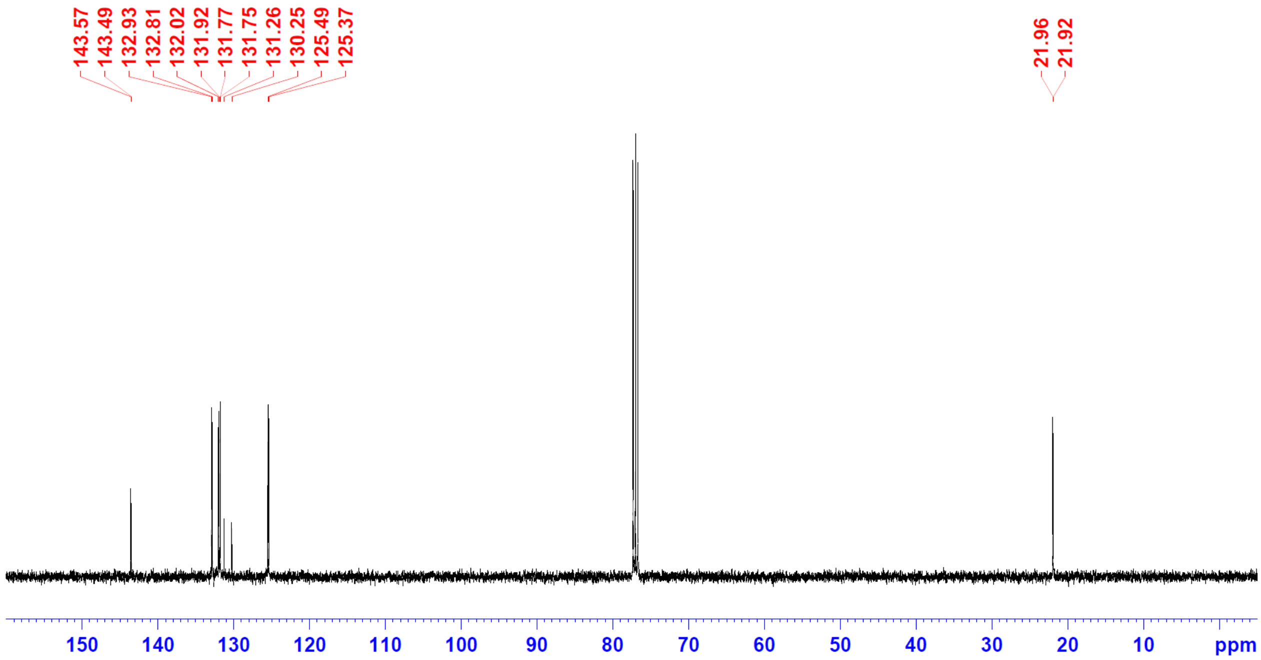
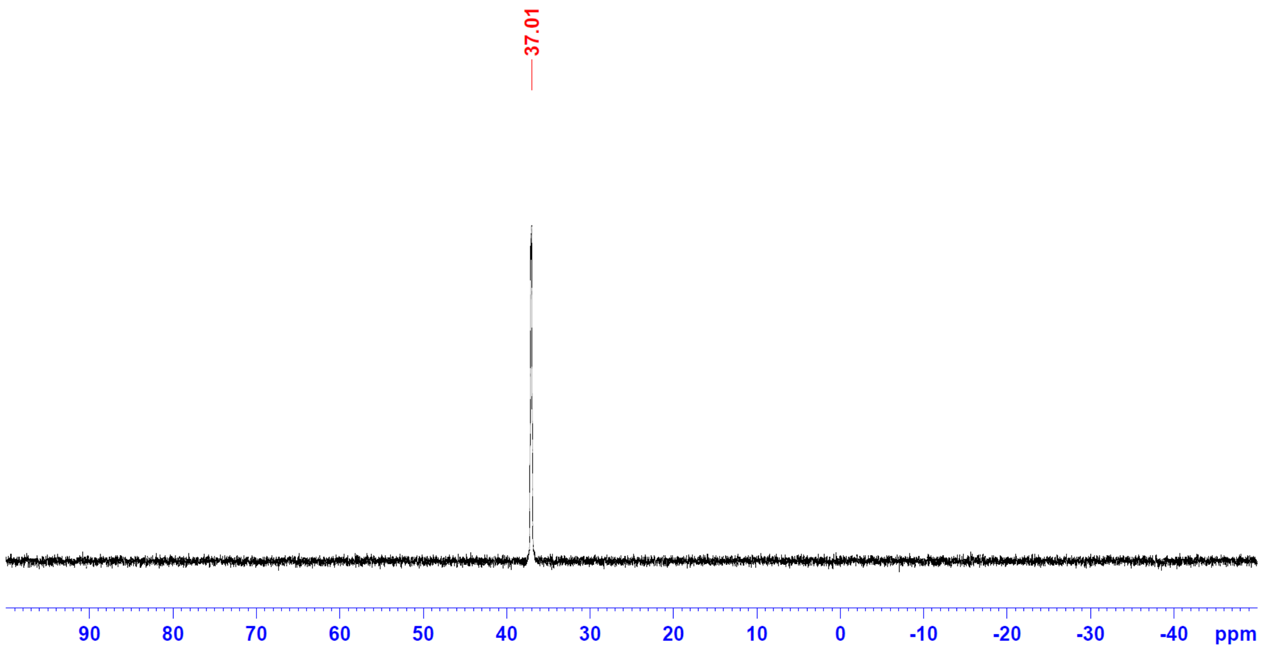
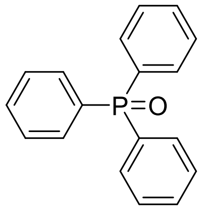


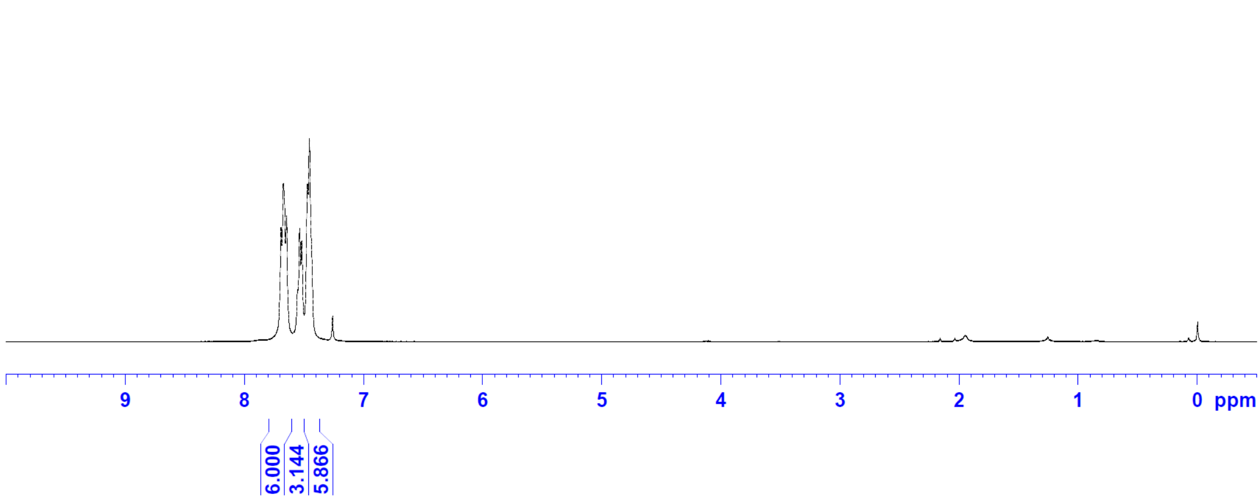
^{31}P-NMR (160 MHz, $CDCl_3$) chart of **2c**



[1]H-NMR (400 MHz, $CDCl_3$) chart of **2d**



2d



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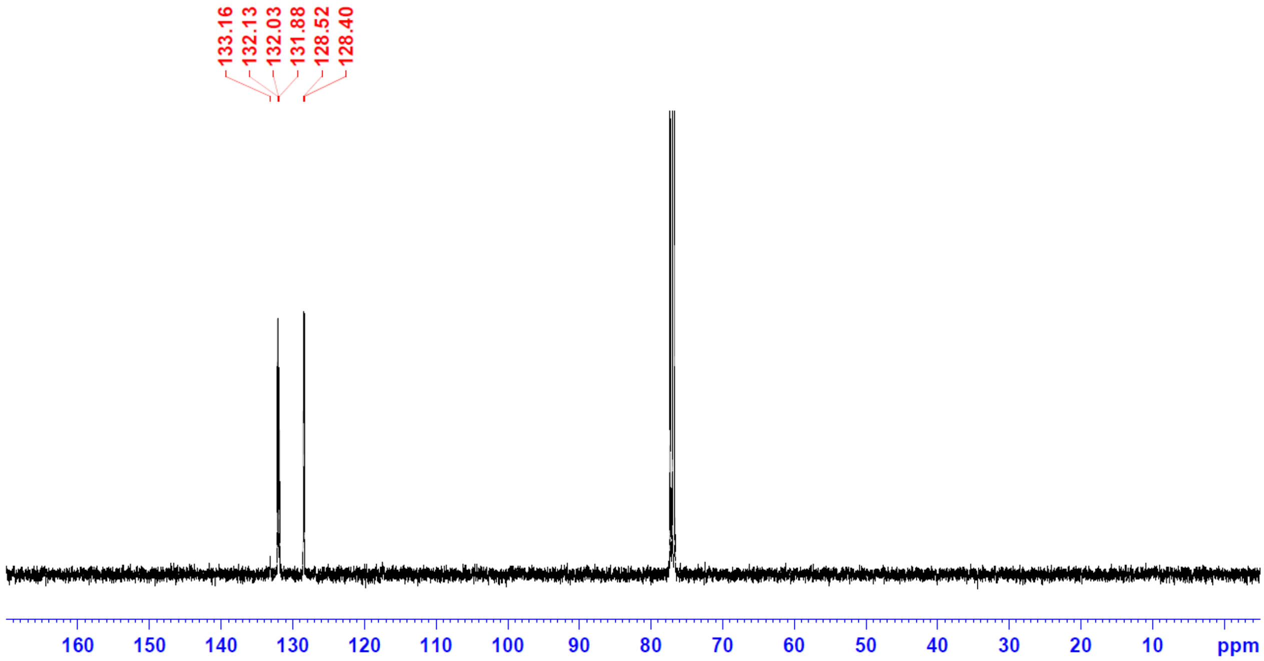

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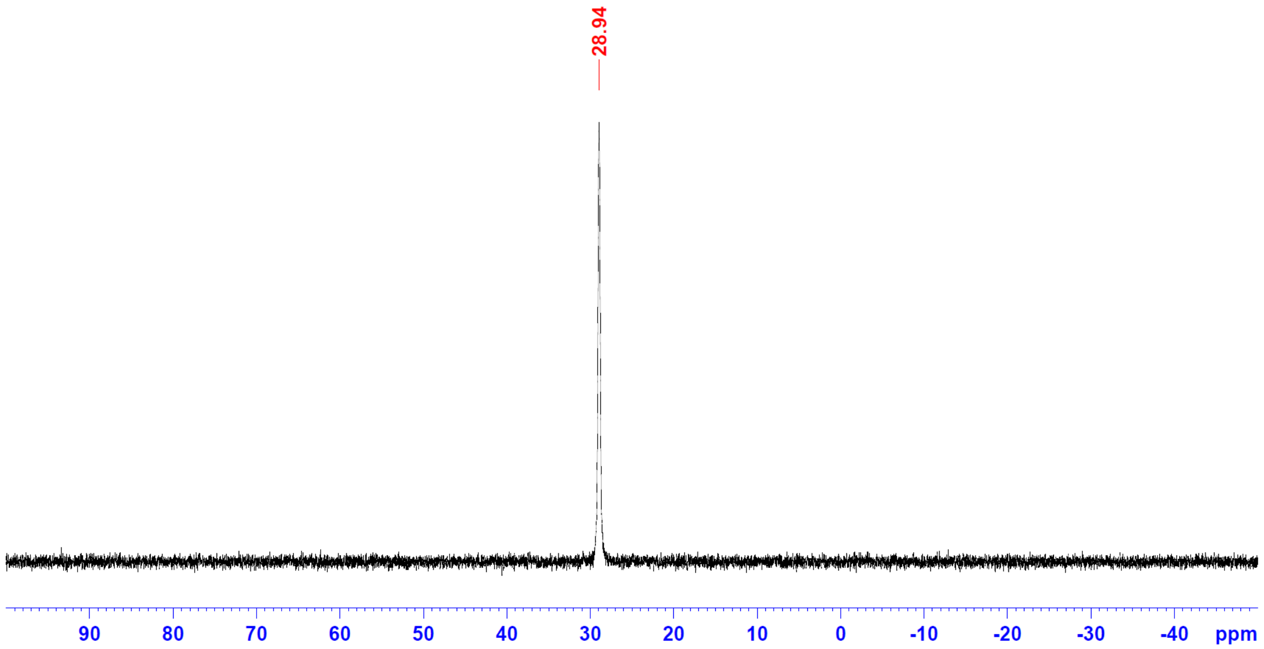
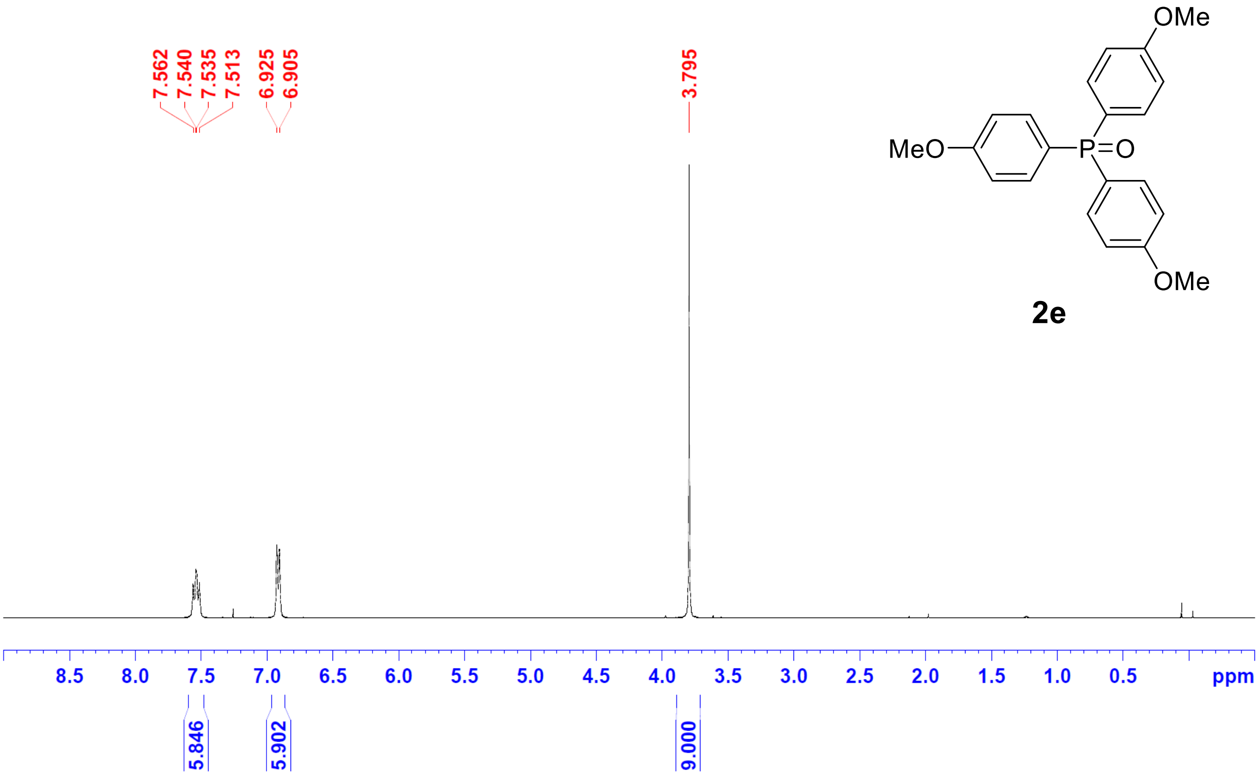


[1]H-NMR (400 MHz, $CDCl_3$) chart of **2e**



2e

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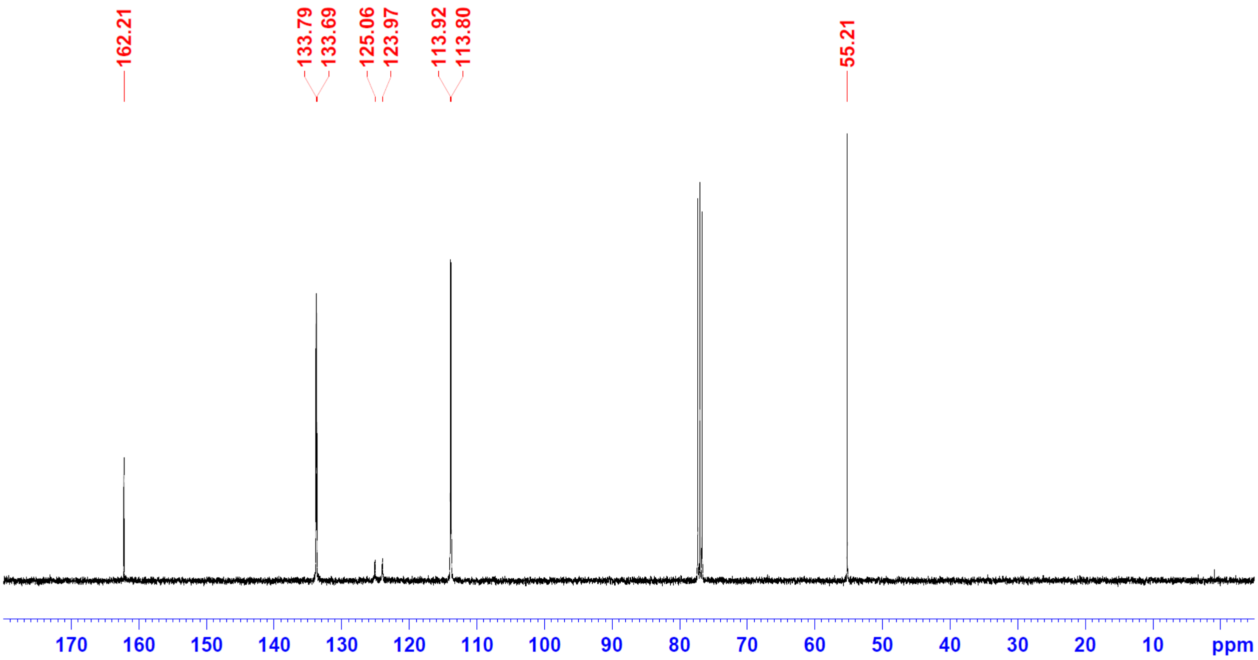

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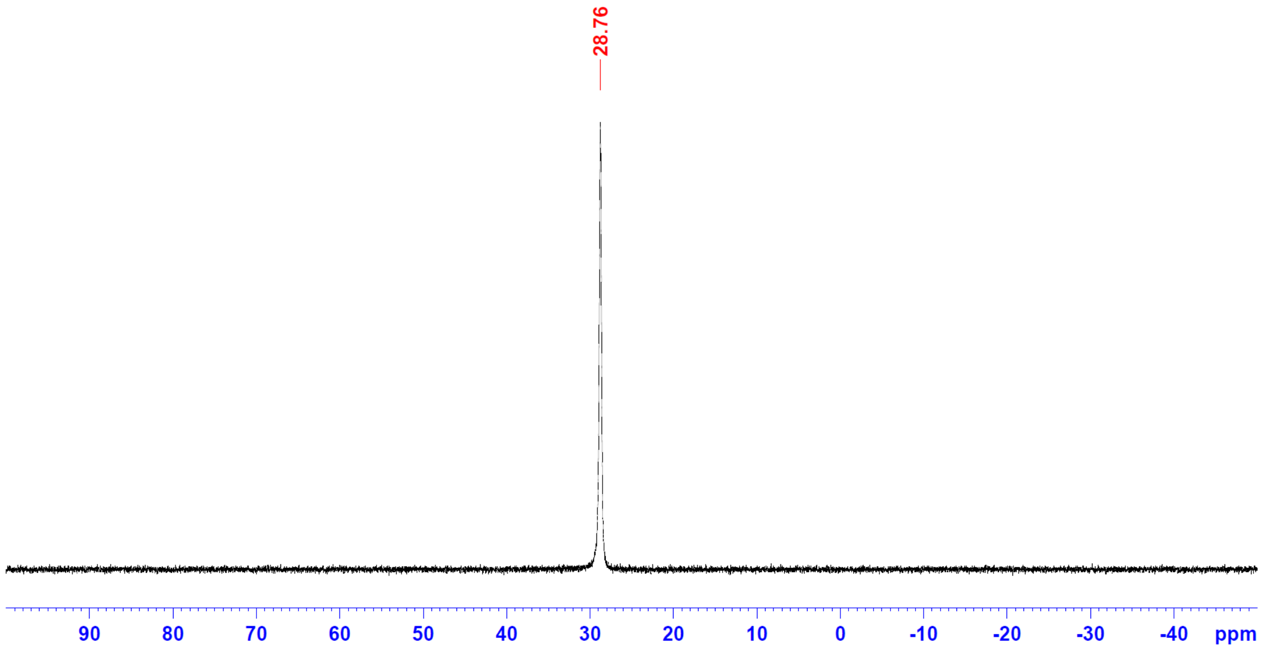
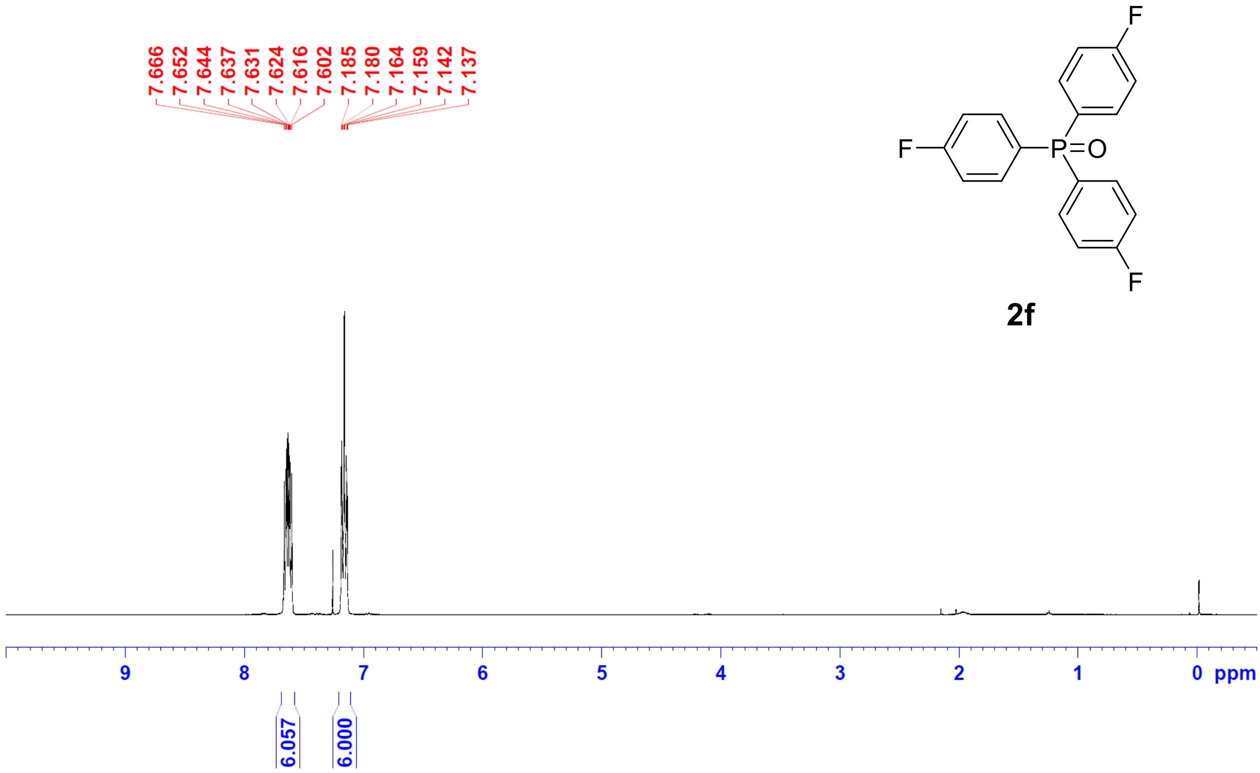
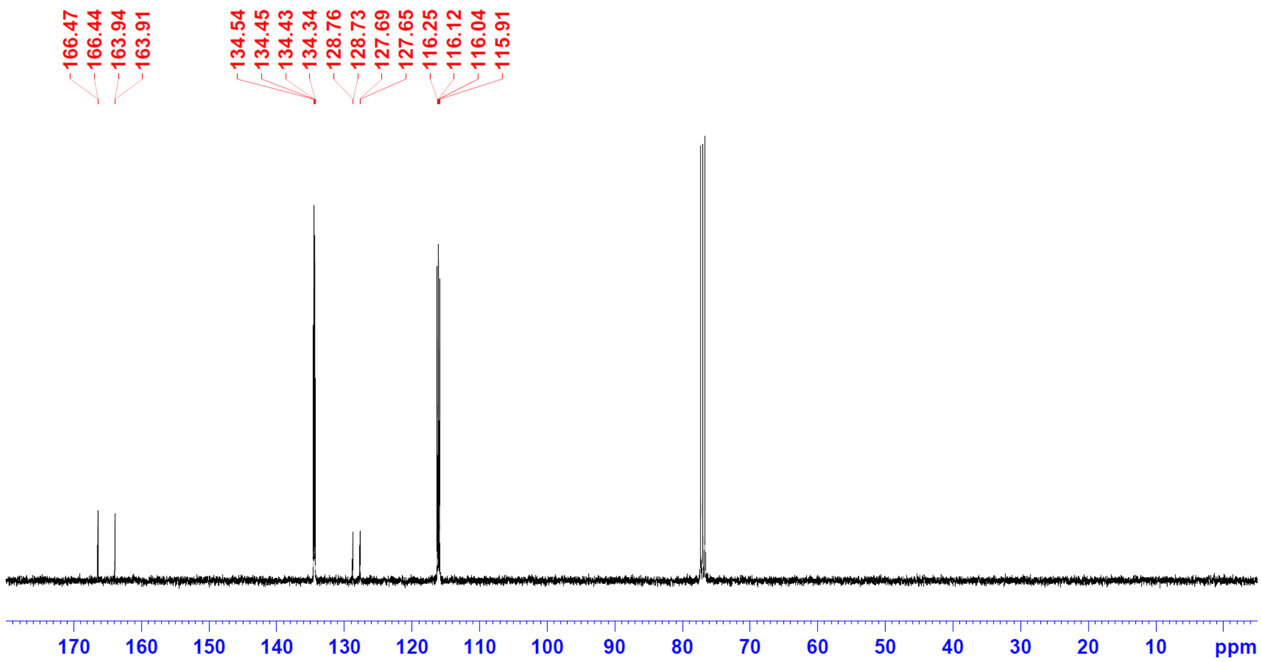


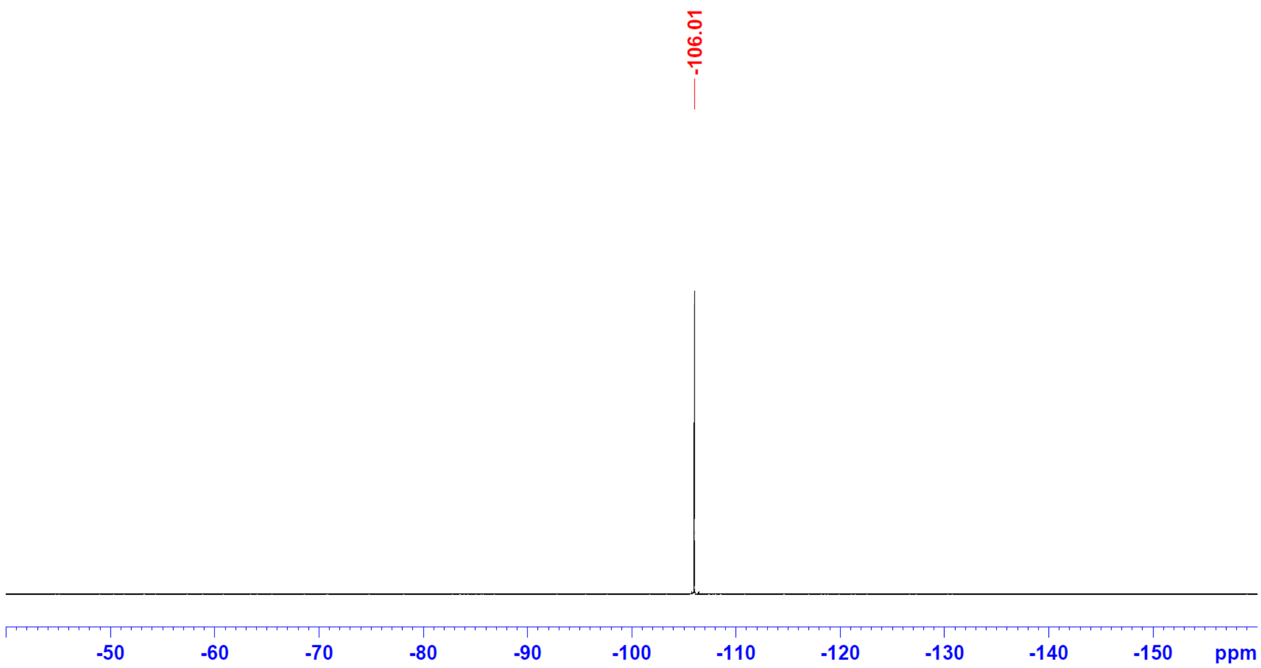
^{1}H-NMR (400 MHz, $CDCl_3$) chart of **2f**



^{13}C-NMR (100 MHz, $CDCl_3$) chart of **2f**



^{19}F-NMR (376 MHz, $CDCl_3$) chart of **2f**



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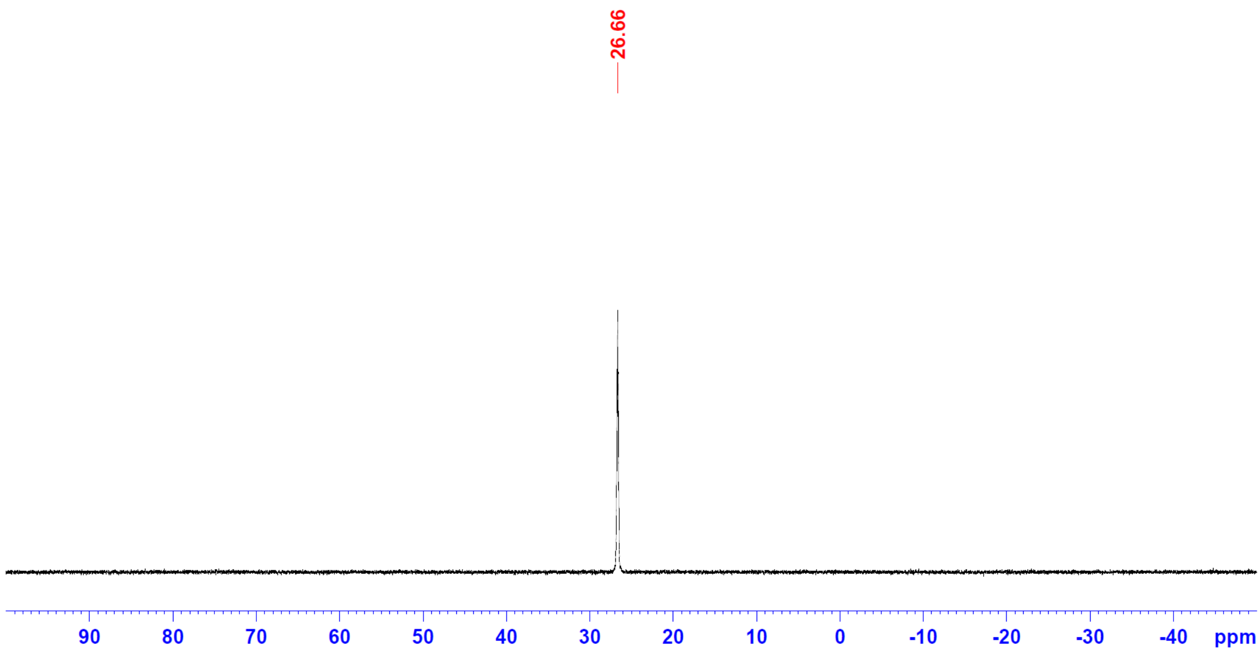
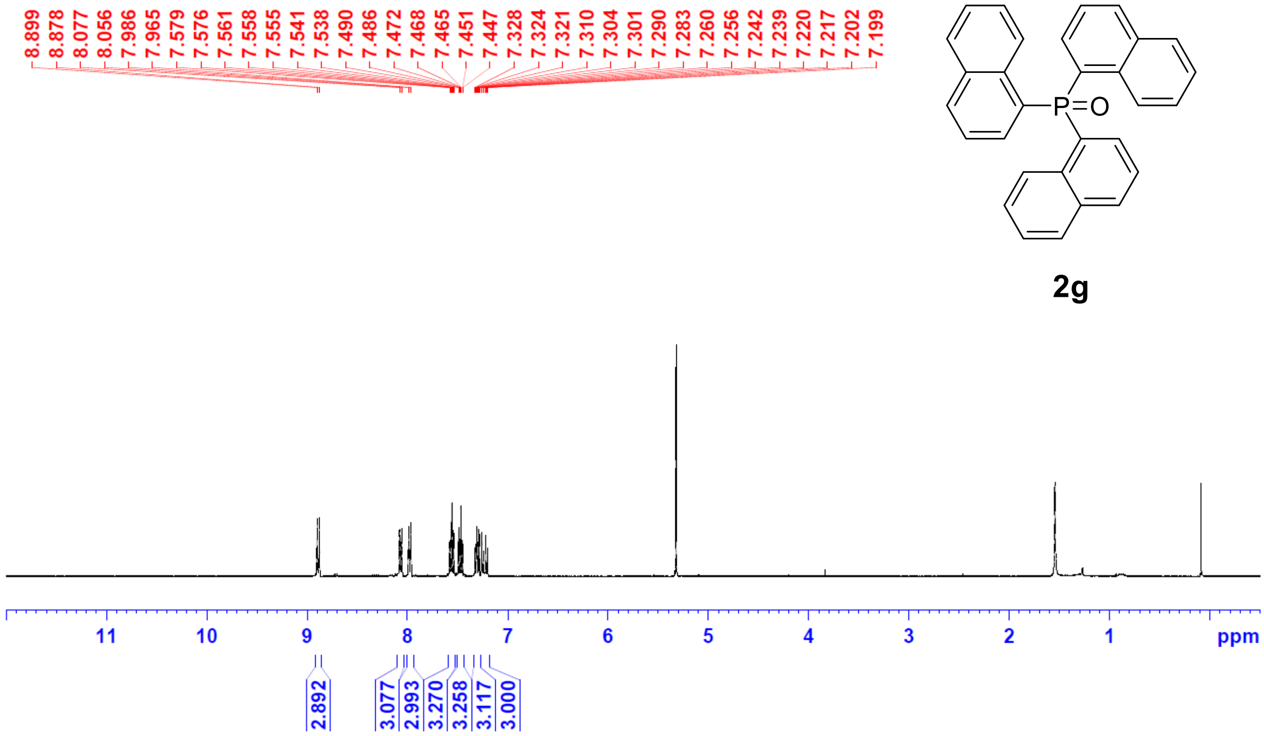


[1]H-NMR (400 MHz, CD_2Cl_2) chart of **2g**



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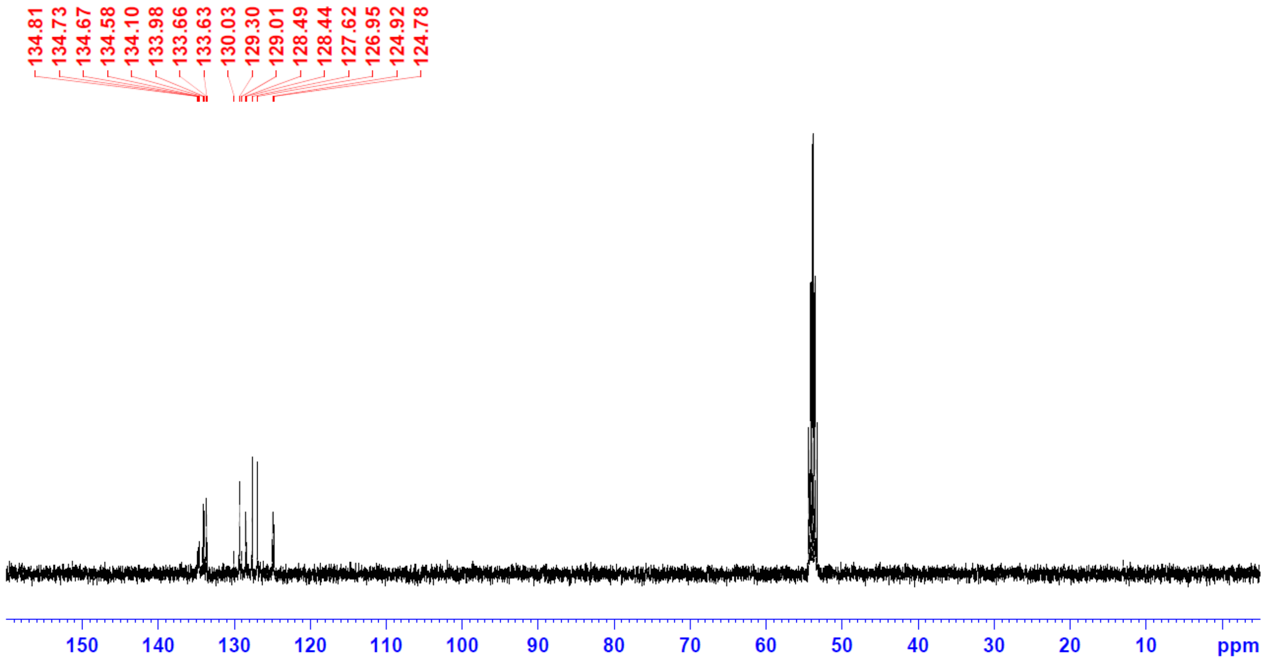

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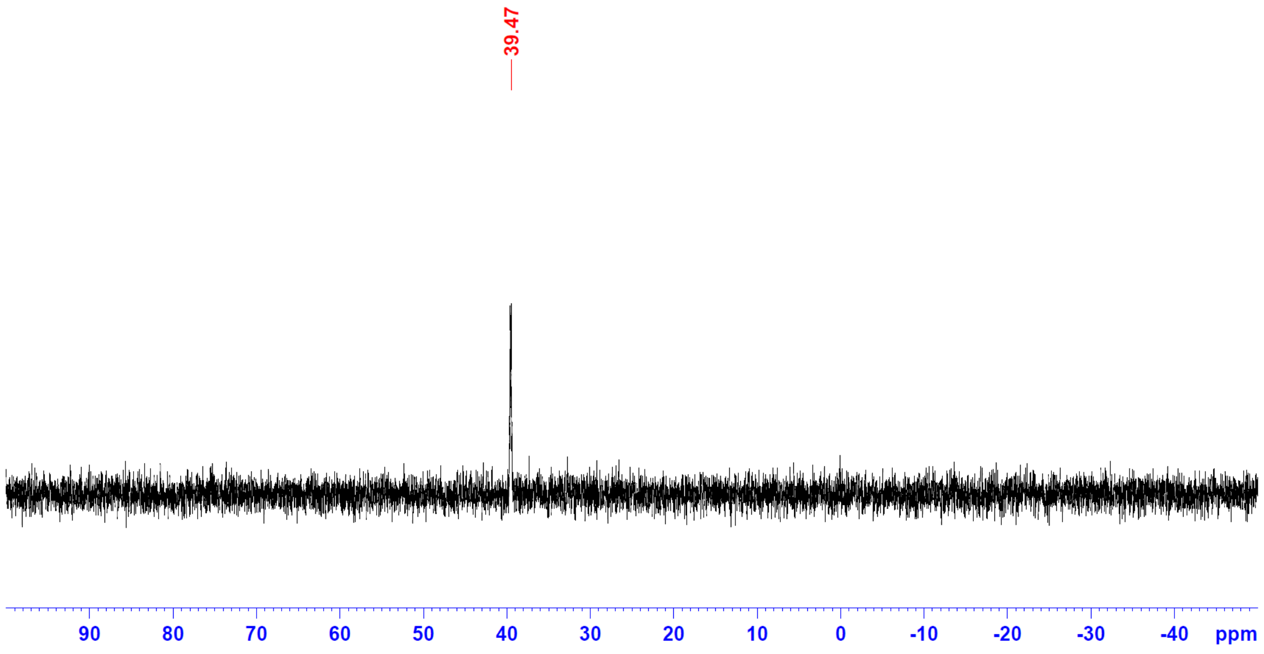
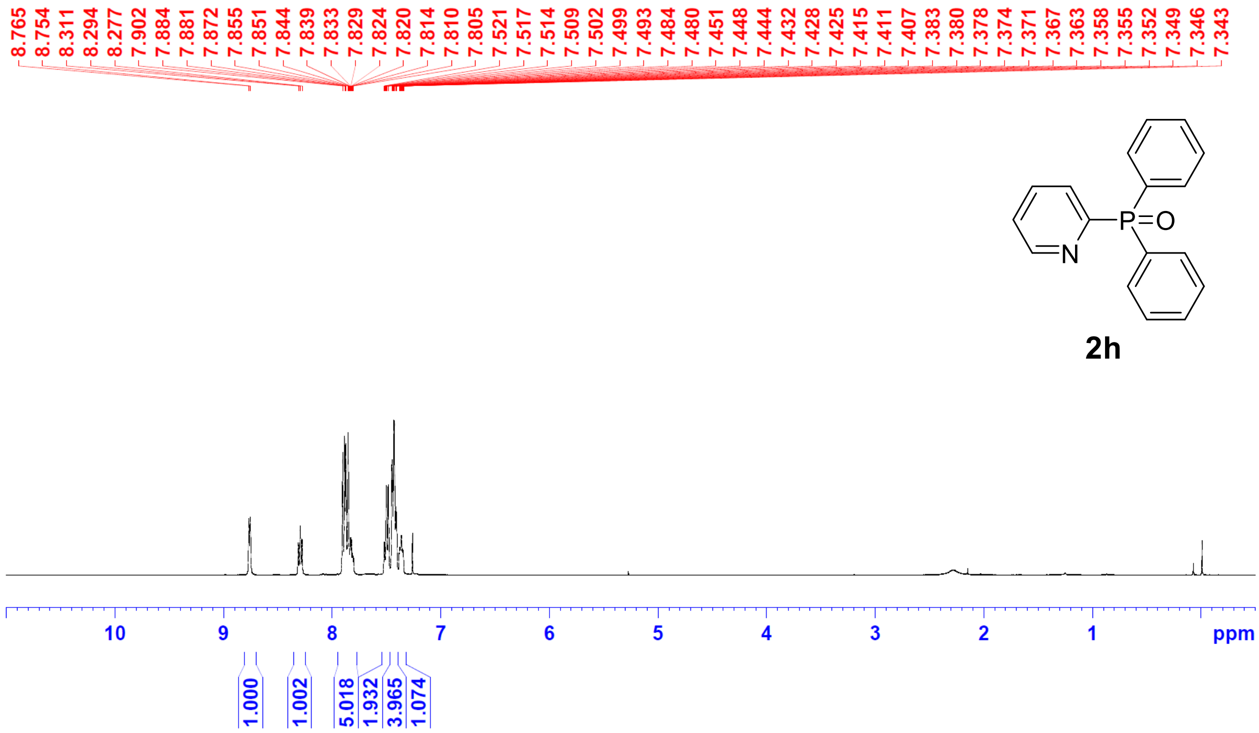


^{1}H-NMR (400 MHz, $CDCl_3$) chart of **2h**



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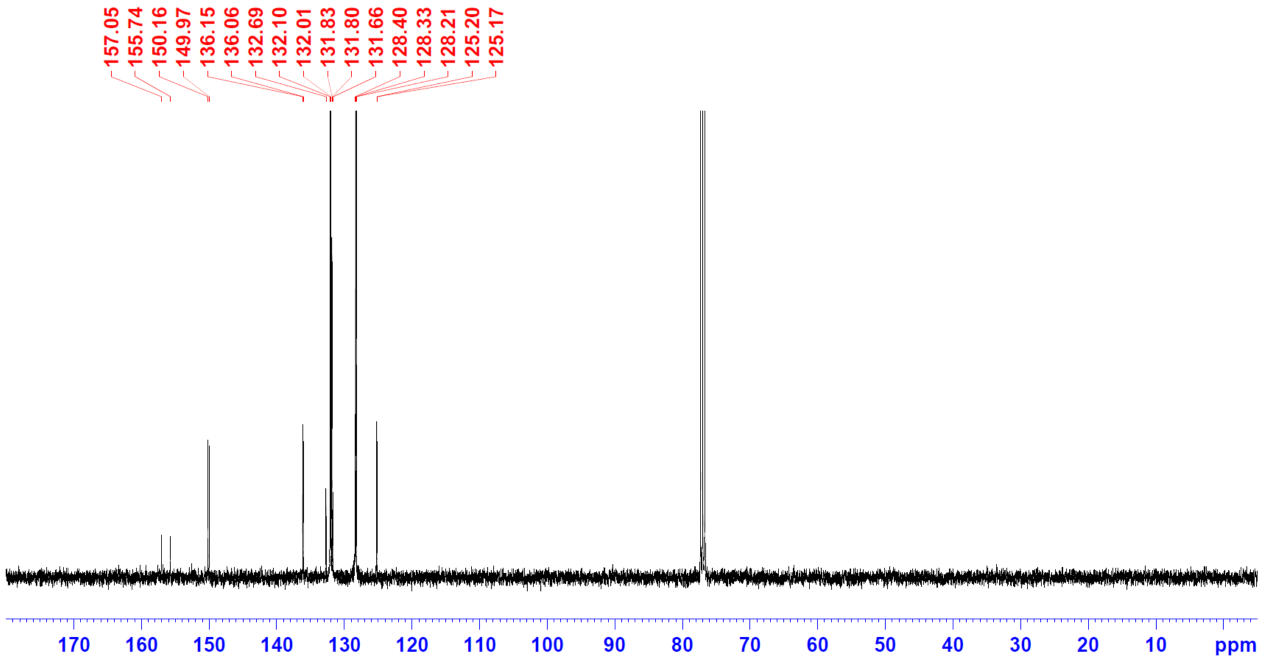

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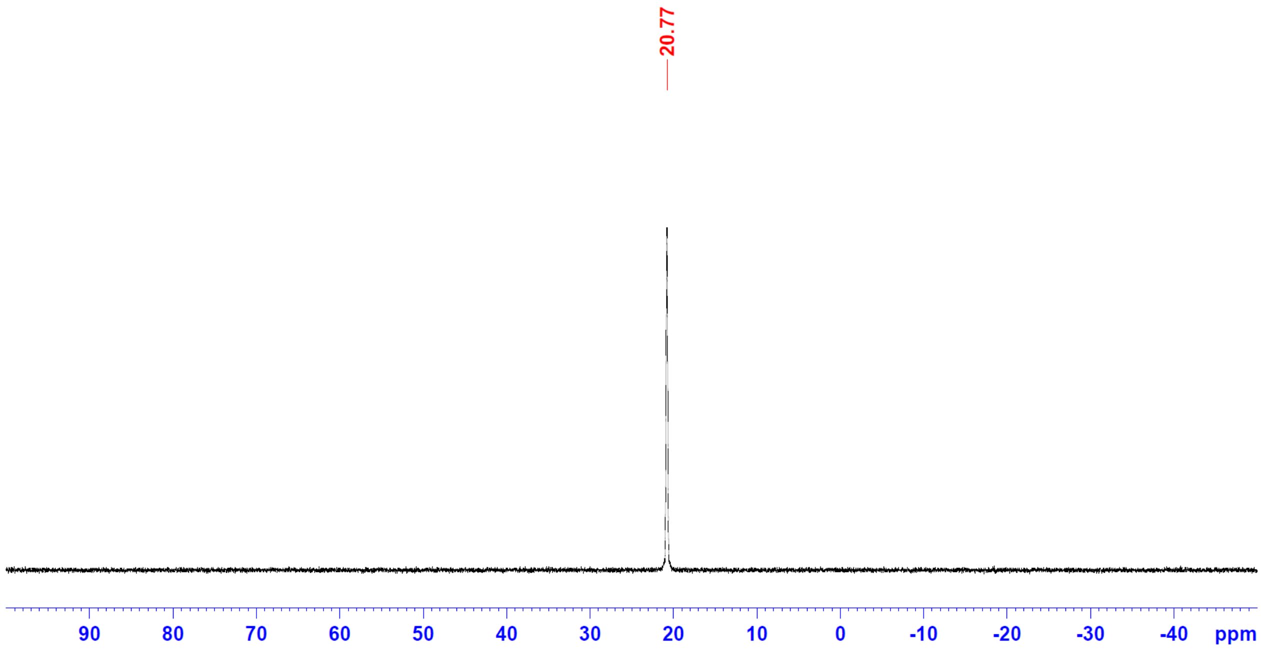

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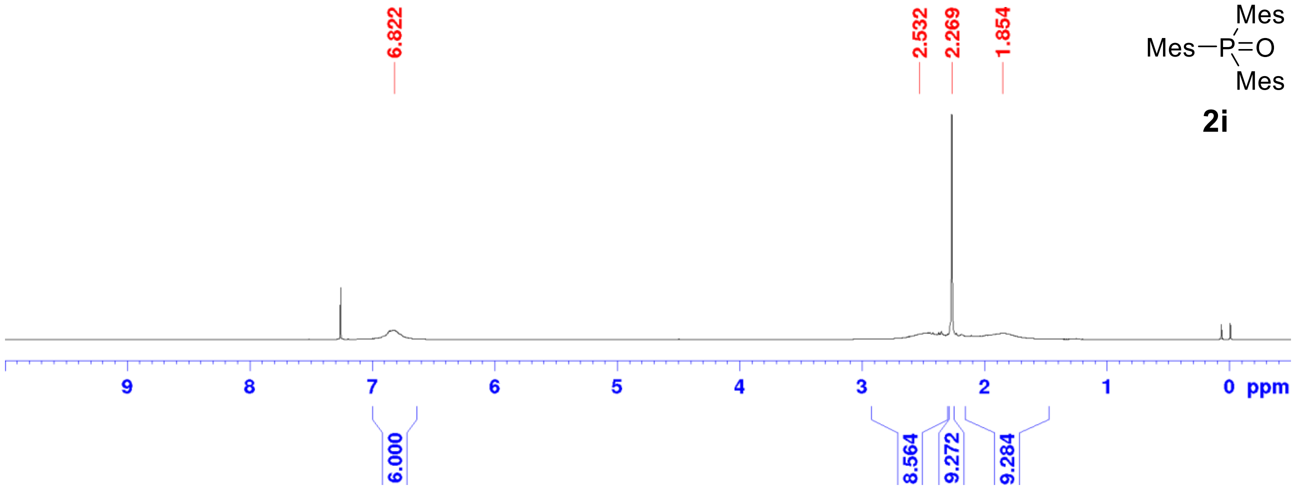

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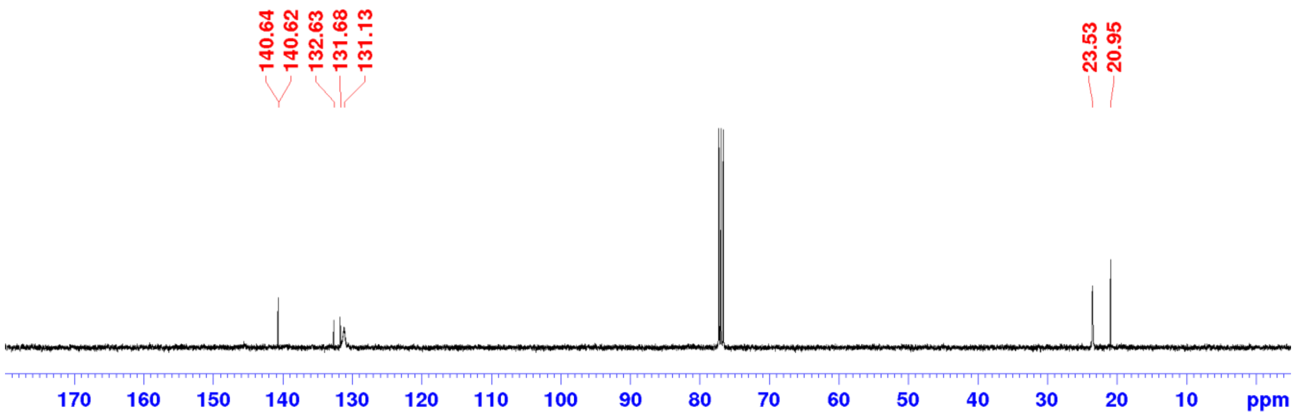

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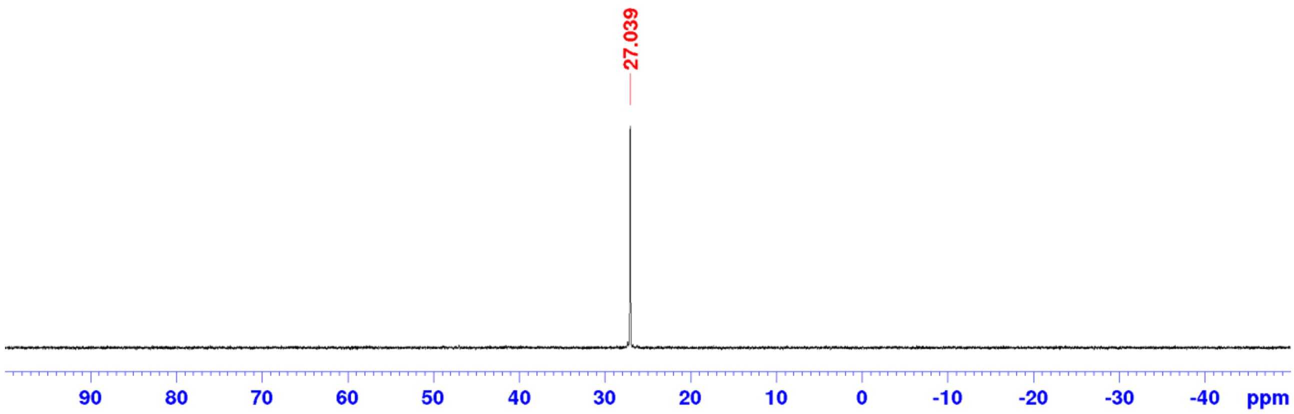

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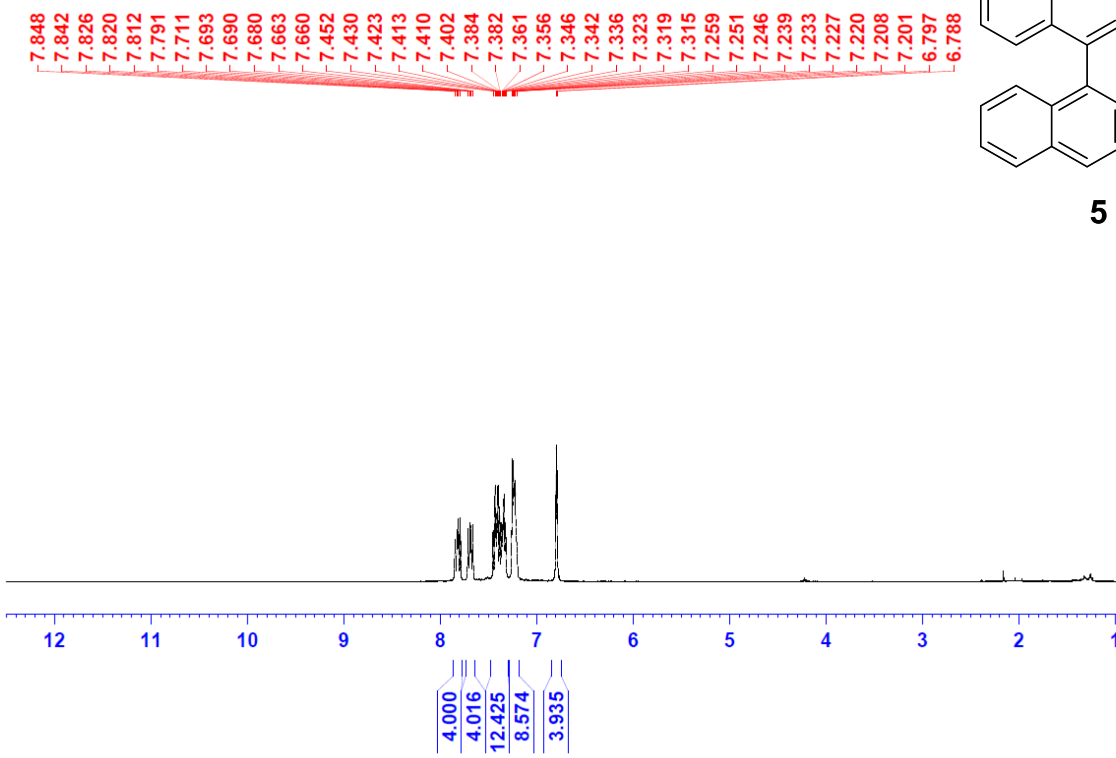

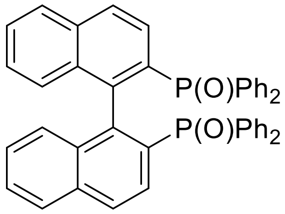

5

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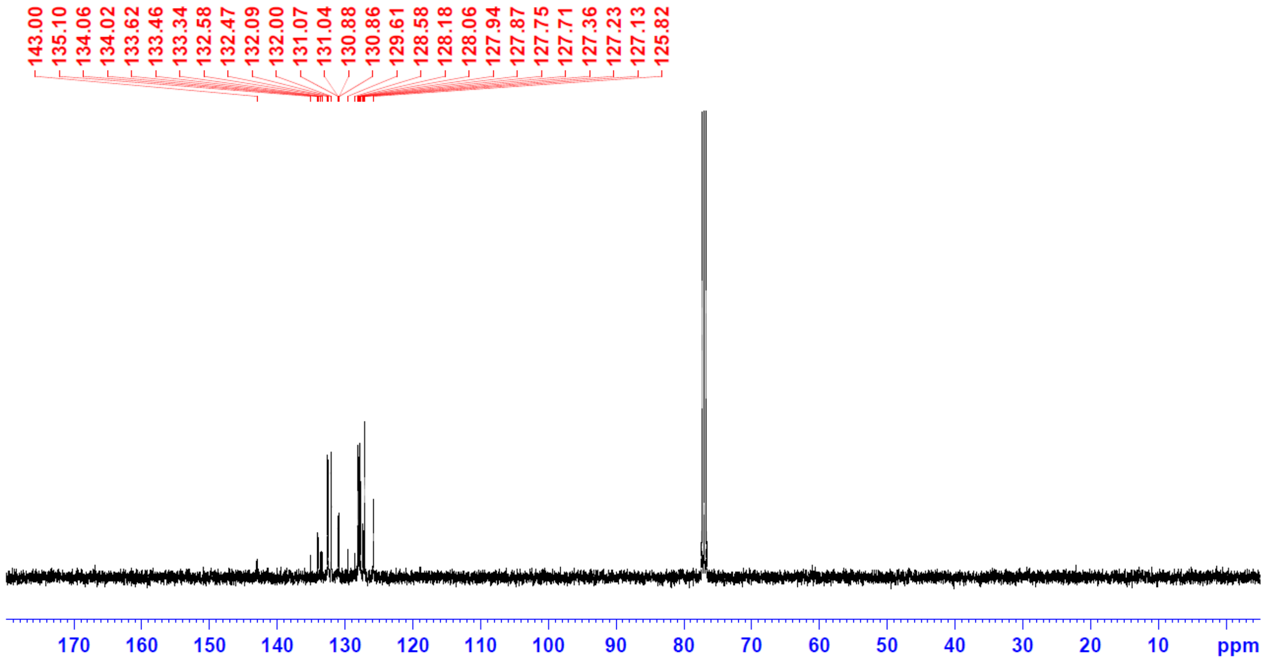

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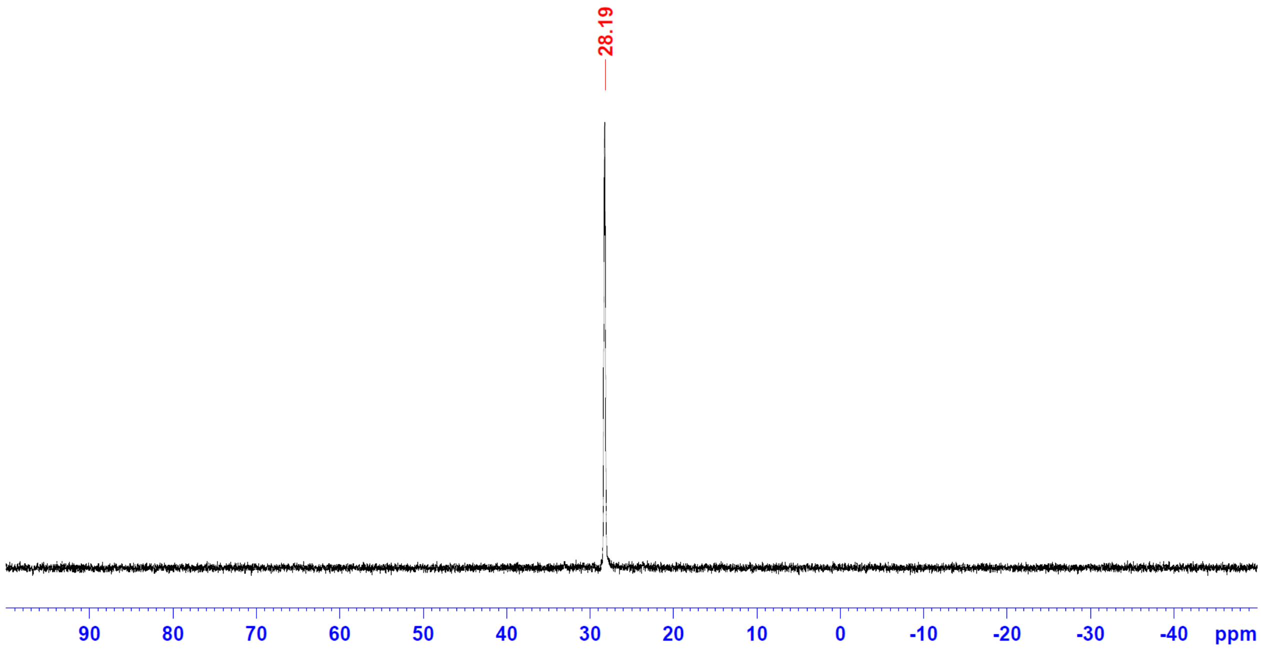
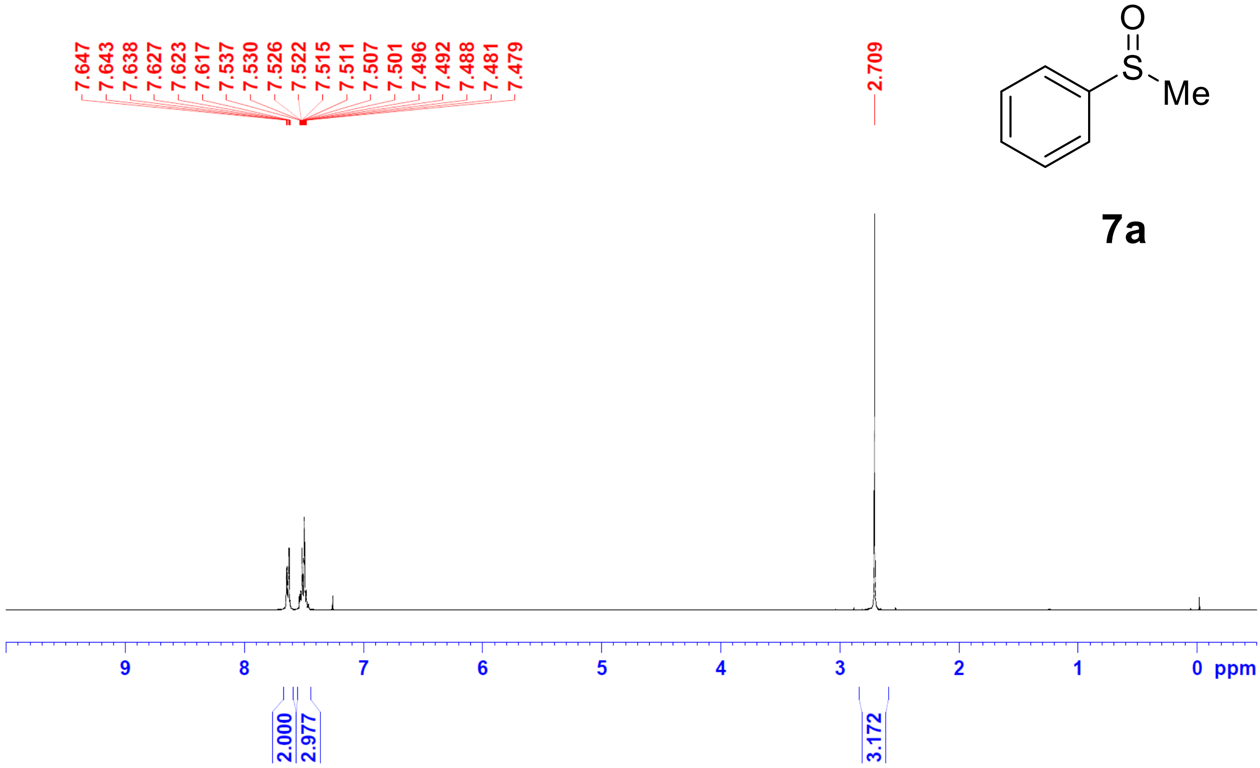
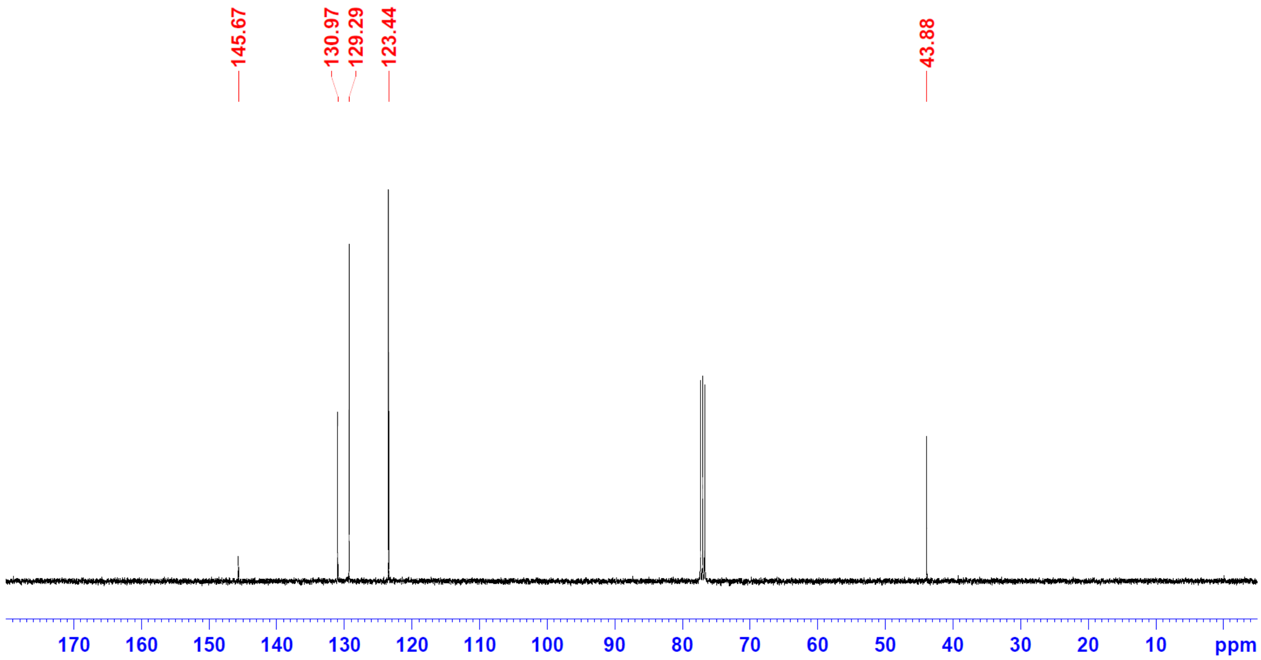


^{1}H-NMR (400 MHz, $CDCl_3$) chart of **7a**



7a

^{13}C-NMR (100 MHz, $CDCl_3$) chart of **7a**



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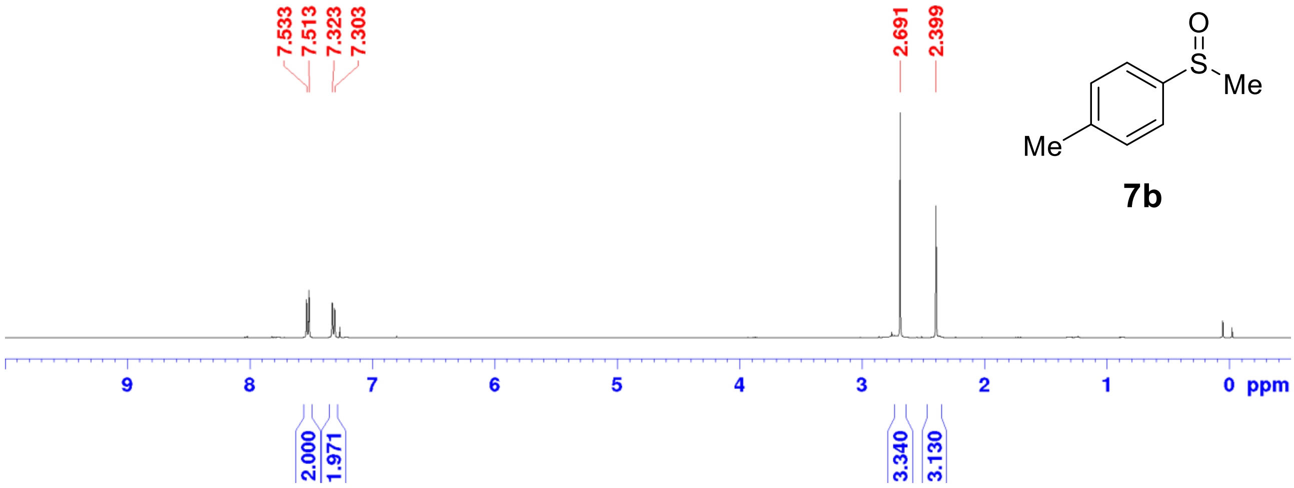

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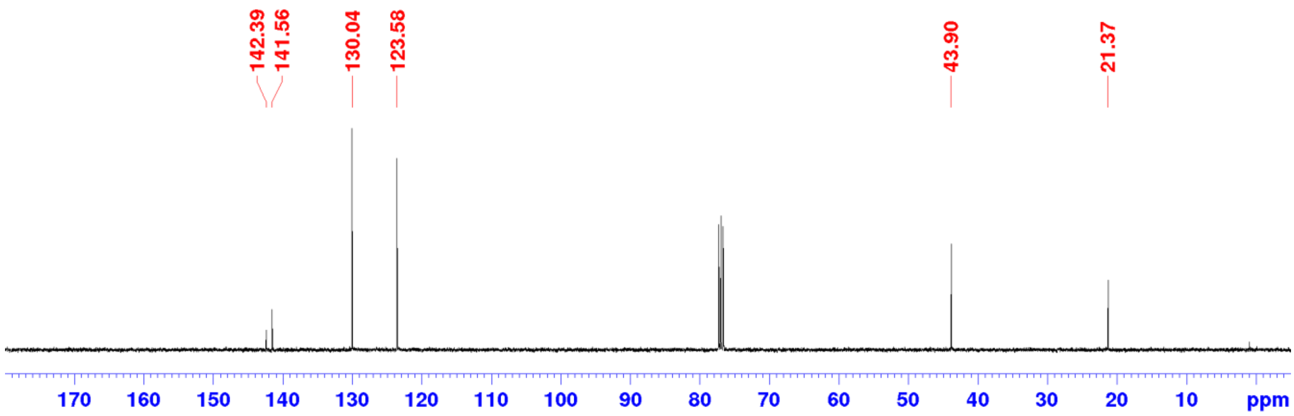

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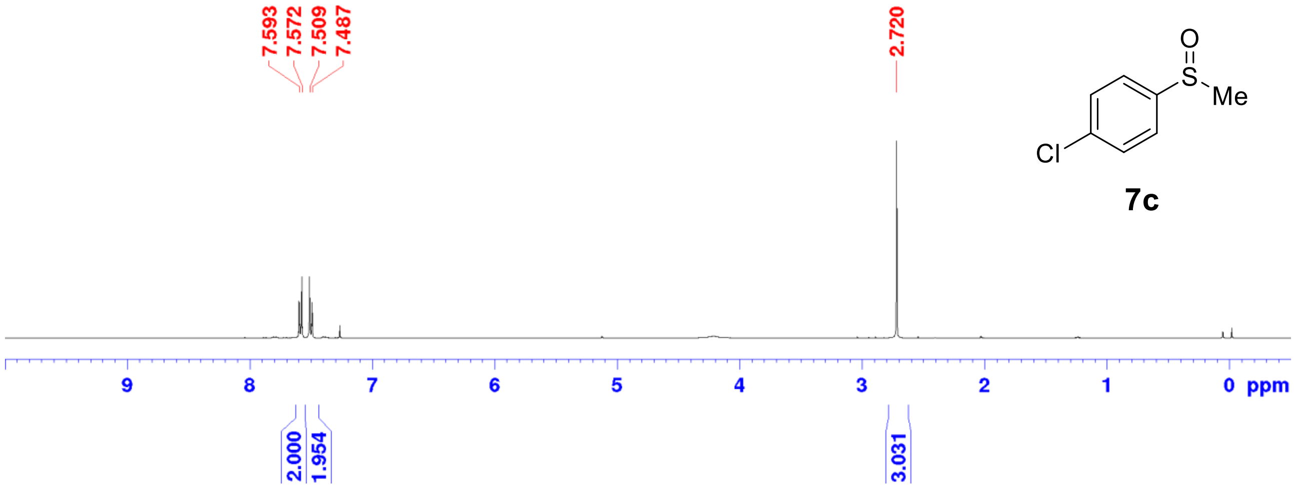

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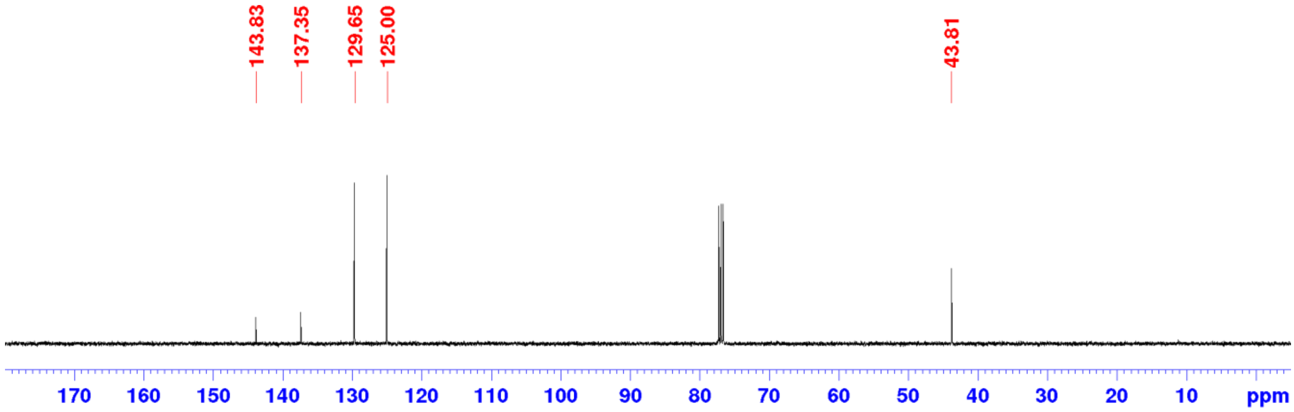

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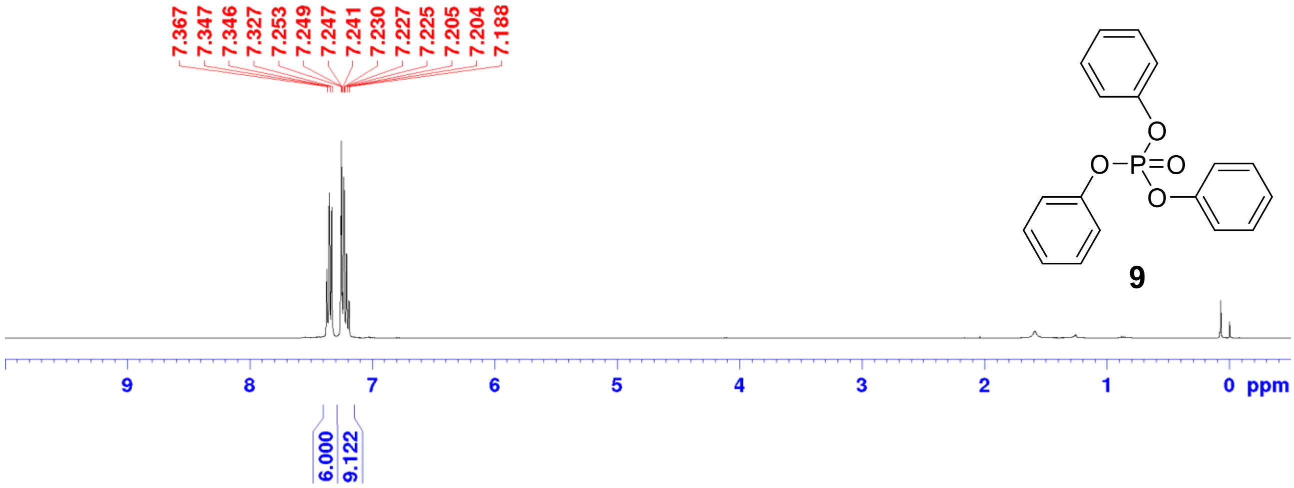

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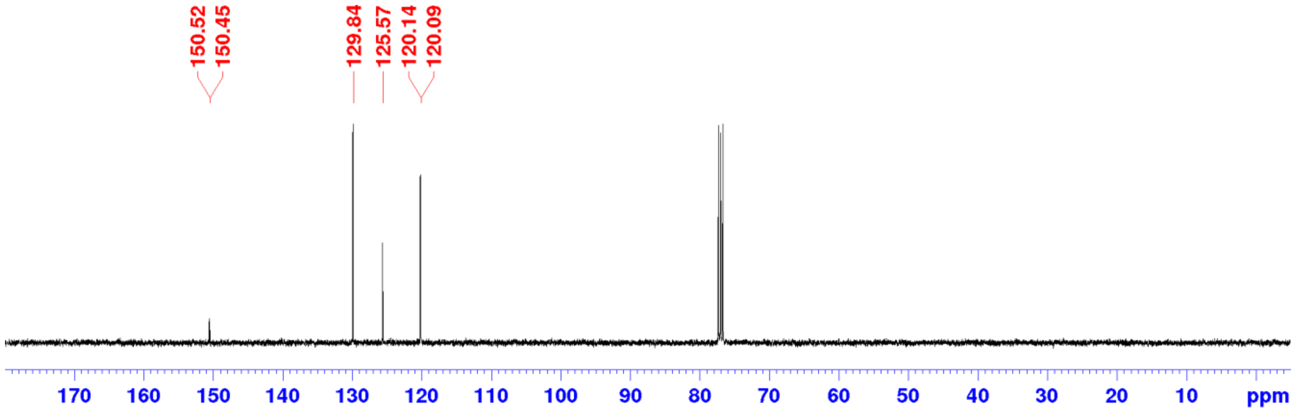
[13]C-NMR (100 MHz, $CDCl_3$) chart of **9**



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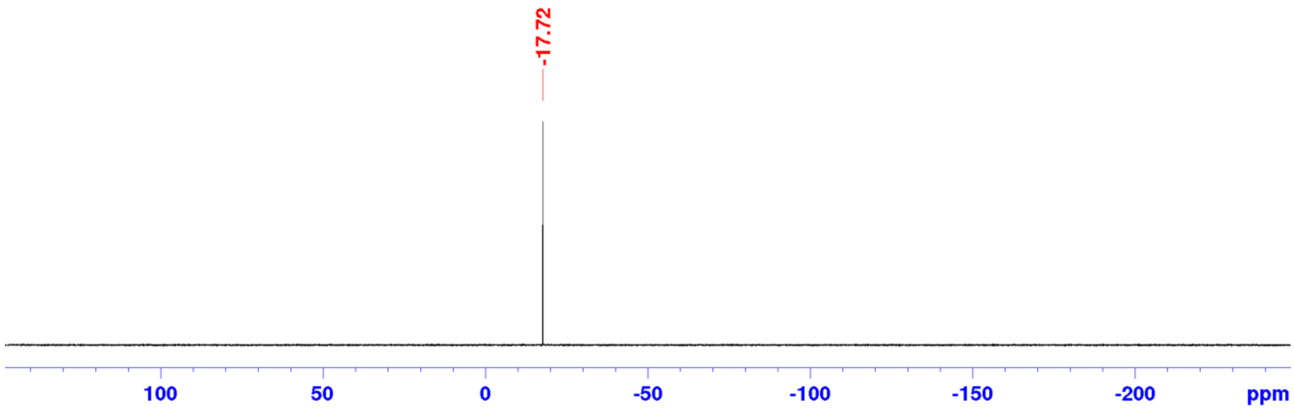
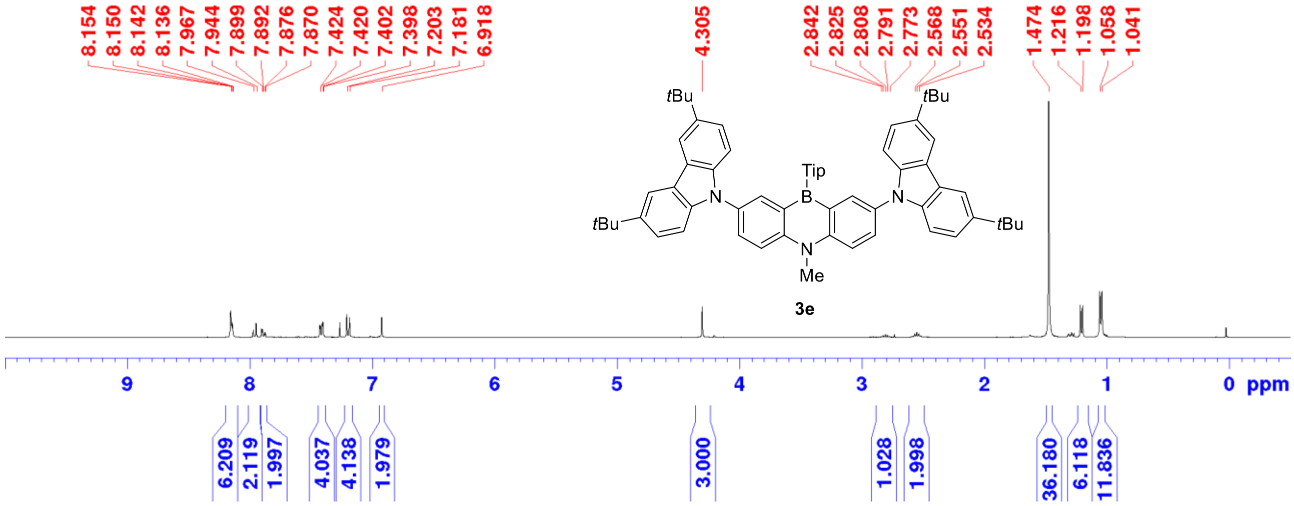


[1]H-NMR (400 MHz, $CDCl_3$) chart of **3e**



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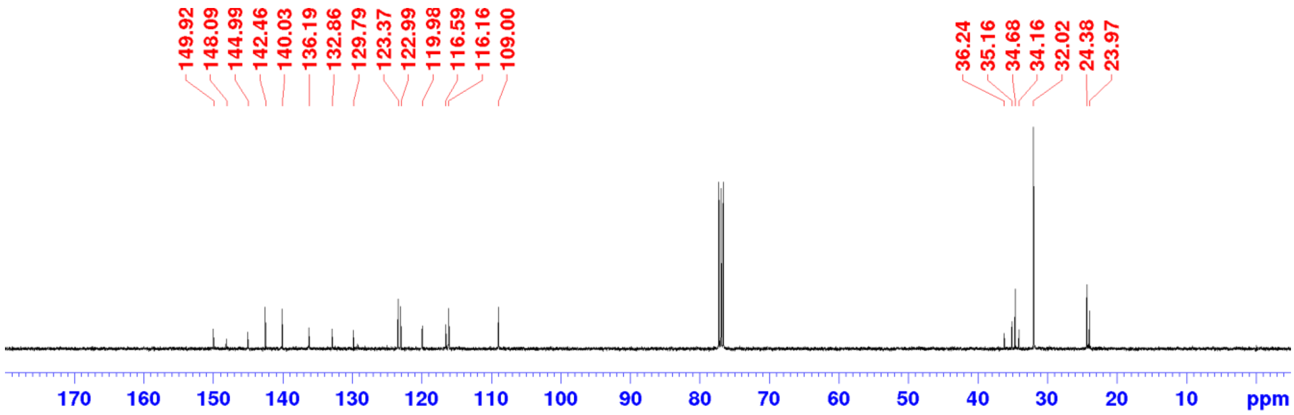

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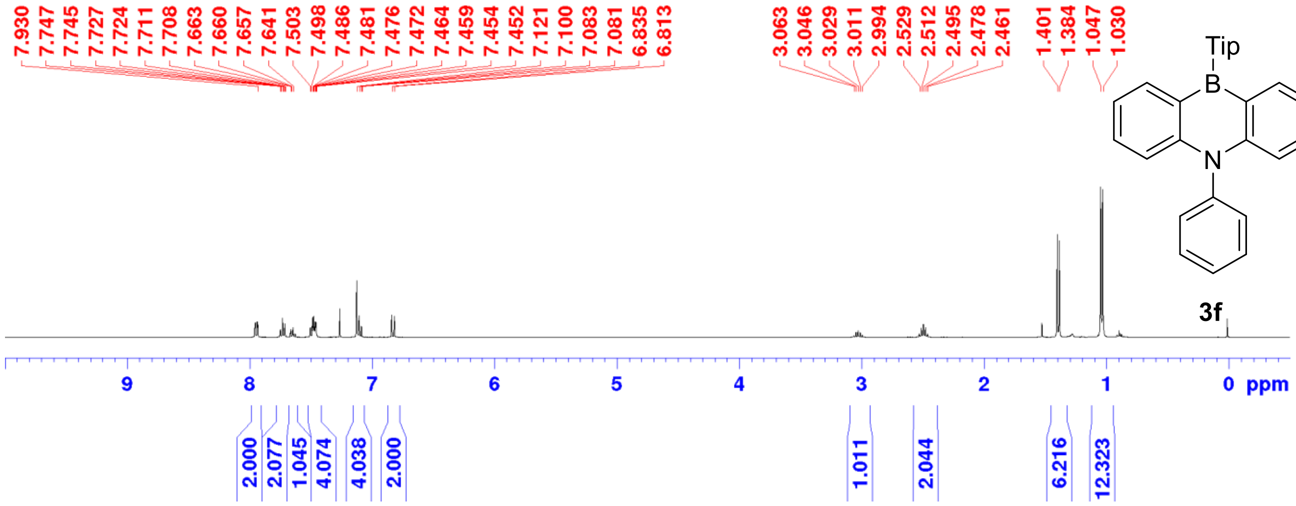

[13]C-NMR (100 MHz, $CDCl_3$) chart of **3f**