Supporting Information

α-Dicationic Chelating Phosphines: Synthesis and Application to the Hydroarylation of Dienes

Lianghu Gu, Lawrence M. Wolf, Adam Zieliński, Walter Thiel and Manuel Alcarazo

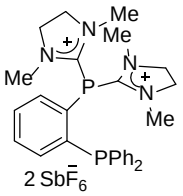
e-mail: malcara@gwdg.de

Table of Contents

Experimental procedures:

General: All reactions were carried out in flame-dried glassware under Ar. All solvents were purified by distillation over the appropiate drying agents and were transferred under Ar. IR: Nicolet FT-7199 spectrometer, wavenumbers in cm^{-1}. MS (EI): Finnigan MAT 8200 (70 eV), ESIMS: Finnigan MAT 95, accurate mass determinations: Bruker APEX III FT-MS (7 T magnet). NMR: Spectra were recorded on a Bruker AV 600, AV 400 or DPX 300; ^{1}H and ^{13}C chemical shifts (δ) are given in ppm relative to TMS, coupling constants (*J*) in Hz. Solvent signals were used as references and the chemical shifts converted to the TMS scale. Column chromatographies were performed on Merck 60 silica gel (40-63 μm), and for thin-layer chromatography (TLC) analyses Merck silica gel 60 F254 TLC plates were used. All commercially available compounds (ABCR, Acros, Aldrich, Fischer) were used as received. 2-(diphenylphosphino)phenylphosphine **3**[1], 2-Chloro-1,3-dimethylimidazolidinium tetrafluoroborate **4**[2], 2-diphenylphosphine-2'-iodo-6,6'-dimethyl-(1,1'-biphenyl) **6**[3], and $(C_6F_5)_2PCl$[4] were prepared according to literature procedures.

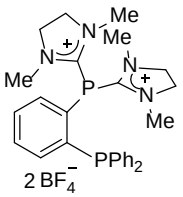
Compound **1a:**



2-Chloro-1,3-dimethylimidazolidinium tetrafluoroborate **4** (150.0 mg, 0.680 mmol) and Et_3N (0.100 ml, 0.710 mmol) were added to a solution of **3** (100.0 mg, 0.340 mmol) in THF (5 ml) and the resulting mixture stirred at 60 ^{o}C overnight. After cooling to r.t., the solvent was filtered and the residue washed with $CHCl_3$ to afford a white solid that was treated with $NaSbF_6$ (352.0 mg, 1.360 mmol) in CH_3CN (5 ml) overnight. Subsequently, the solvent was removed *in vacuo* and the resulting white solid extracted with CH_2Cl_2 (3 × 10 ml). The combined organic phases were evaporated *in vacuo* affording **1** as a white solid (234.9 mg, 72%). Colourless crystals suitable for X−ray crystallography were obtained from a CH_2Cl_2/Et_2O solution at -20 ^{o}C.

^{1}H NMR (CD_3CN, 400 MHz): δ = 7.76 – 7.68 (m, 3H), 7.53 – 7.45 (m, 6H), 7.42 – 7.38 (m, 1H), 7.34 – 7.30 (m, 4H), 3.84 - 3.80 (m, 8H), 2.98 ppm (s, 12H); ^{13}C NMR (CD_3CN, 100 MHz): δ = 164.4 (dd, *J* = 47.5 Hz, *J* = 18.1 Hz), 144.3 (dd, *J* = 30.0 Hz, *J* = 4.9 Hz), 137.1 (d, *J* = 7.2 Hz), 136.6 (d, *J* = 8.4 Hz), 135.0, 134.4 (d, *J* = 18.6 Hz), 134.0 (dd, *J* = 6.0 Hz;1.0 Hz), 133.2, 131.3, 130.4, (d, *J* = 7.3 Hz), 127.3 (dd, *J* = 40.6 Hz; 4.2 Hz), 53.4, 36.8 ppm (d, *J* = 8.7 Hz); ^{31}P NMR (CD_3CN, 121 MHz): δ = -10.7 (d, J_{P-P} = 212.4 Hz), -46.1 ppm (d, J_{P-P} = 212.4 Hz); ^{19}F NMR (CD_3CN, 376 MHz): δ = -124.0 ppm (sextet, $J_{F-121Sb}$ = 1945 Hz; octet, $J_{F-123Sb}$ = 1071 Hz); HRMS *calcd.* for $C_{28}H_{34}N_4SbF_6P_2^+$: 723.119040; *found*: 723.119040; IR $\tilde{\nu}$ = 422, 456, 518, 653, 699, 745, 767, 934, 998, 1090, 1107, 1300, 1335, 1412, 1434, 1445, 1521, 1576, 3103 cm^{-1}.

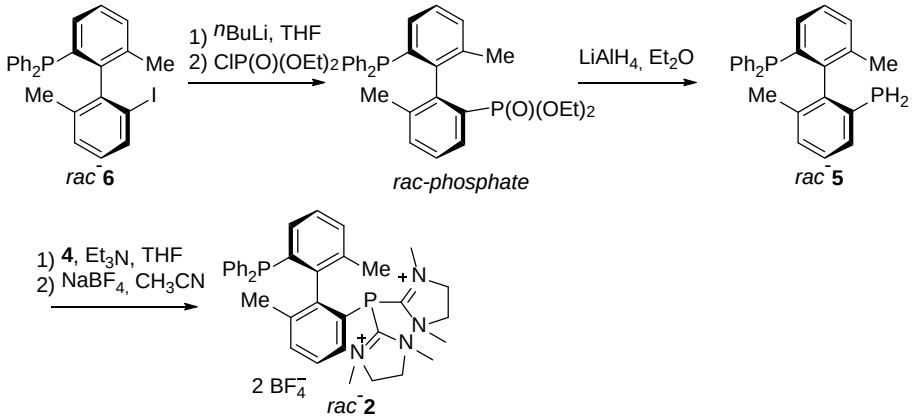
Compound **1b:**

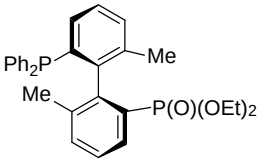


2-Chloro-1,3-dimethylimidazolidinium tetrafluoroborate **4** (150.0 mg, 0.680 mmol) and Et_3N (0.100 ml, 0.710 mmol were added to a solution of **3** (100.0 mg, 0.340 mmol) in THF (5 ml) and the resulting mixture stirred at 60 ^{o}C overnight. After cooling to r.t., the solvent was filtered and the residue washed with $CHCl_3$ to afford a white solid that was treated with $NaBF_4$ (149.6 mg, 1.360 mmol) in CH_3CN (5 ml) overnight. Subsequently, the solvent was removed *in vacuo* and the resulting white solid extracted with CH_2Cl_2 (3 × 20 ml). The combined organic phase was evaporated *in vacuo* to afford **1b** as a white solid (146.3 mg, 65%).

^{1}H NMR (CD_3CN, 400 MHz): δ = 7.76 – 7.68 (m, 3H), 7.53 – 7.45 (m, 6H), 7.42 – 7.38 (m, 1H), 7.34 – 7.30 (m, 4H), 3.84 - 3.80 (m, 8H), 2.98 ppm (s, 12H); ^{13}C NMR (CD_3CN, 100 MHz): δ = 164.4 (dd, *J* = 47.5 Hz; 18.0 Hz), 144.3 (dd, *J* = 35.6 Hz; 5.1 Hz), 137.1 (d, *J* = 7.8 Hz), 136.6 (d, *J* = 8.2 Hz), 135.2 (d, *J* = 1.4 Hz), 134.5, 134.3, 134.0 (dd, *J* = 6.0 Hz; 1.0 Hz), 133.2, 131.3, 130.4, (d, *J* = 7.3 Hz), 127.3 (dd, *J* = 39.5 Hz; 3.1 Hz), 53.4, 36.8 ppm (d, *J* = 8.7 Hz); ^{31}P NMR (CD_3CN, 121 MHz): δ = -12.3 (d, $J_{P\text{-}P}$ = 211.6 Hz), -47.6 ppm (d, $J_{P\text{-}P}$ = 212.6 Hz); ^{11}B NMR (CD_3CN, 96 MHz): δ = – 1.2 ppm; ^{19}F NMR (CD_3CN, 282 MHz): δ = -151.8 ppm; HRMS *calcd.* for $C_{28}H_{34}N_4BF_4P_2^+$: 575.228360; *found* 575.228243; IR $\tilde{\nu}$ = 425, 457, 522, 653, 699, 741, 762, 936, 998, 1094, 1111, 1300, 1337, 1418, 1434, 1445, 1523, 1579, 3105 cm^{-1}.

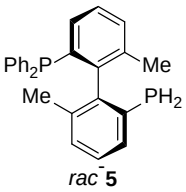
Synthesis of **2**:





Rac-**6** (2.3 g, 4.672 mmol) was dissolved in THF (25 ml) and *n*BuLi (1.6 M in hexanes, 2.92 ml, 4.672 mmol) was added dropwise at -78 °C. After 1h at this temperature a solution of $ClP(O)(OEt)_2$ (0.680 ml, 4.672 mmol) in THF (5 mL) was added dropwise and subsequently the mixture was allowed to warm to r.t. overnight. Then all volatiles were removed *in vacuo* and the crude purified by column chromatography (SiO_2, hexane : EtOAc = 3 : 1) to afford the desired phosphate (1.1 g, 47%).

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.90 (dd, *J* = 15.2 Hz; 7.12 Hz, 1H), 7.38 - 7.34 (m, 1H), 7.32 – 7.18 (m, 14H), 3.99 – 3.12 (m, 4H), 1.97 (s, 3H), 1.27 (s, 3H), 1.15 ppm (q, *J* = 5.8 Hz, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 145.5 (dd, *J* = 33.5 Hz; 4.1 Hz), 143.4 (d, *J* = 8.2 Hz), 143.3 (d, *J* = 9.0 Hz), 139.7 (d, *J* = 13.9 Hz), 138.4 (dd, *J* = 15.3 Hz; 2.3 Hz), 138.0 (d, *J* = 11.4 Hz), 137.0 (d, *J* = 6.5 Hz), 136.9 (d, *J* = 13.4 Hz), 135.4 (d, *J* = 22.7 Hz), 133.9 (d, *J* = 2.9 Hz), 133.0 (d, *J* = 17.1 Hz), 131.7 (d, *J* = 1.8 Hz), 131.1 (d, *J* = 9.2 Hz), 130.5, 129.0, 128.4 (d, *J* = 7.7 Hz), 128.0 (d, *J* = 4.9 Hz), 127.5 (d, *J* = 10.4 Hz), 127.3 (d, *J* = 15.6 Hz), 127.1 (d, *J* = 2.8 Hz), 61.8 (t, *J* = 5.4 Hz), 20.5 (d, *J* = 2.7 Hz), 19.4, 16.4 ppm (dd, *J* = 11.7 Hz; 6.0 Hz); ^{31}P NMR ($CDCl_3$, 121 MHz): δ = 17.7, -16.2 ppm; HRMS *calcd.* for $C_{30}H_{32}O_3P_2Na^+$: 525.171490; *found* 525.171893; IR $\tilde{\nu}$ = 426, 445, 485, 514, 539, 574, 591, 696, 751, 787, 878, 953, 998, 1051, 1090, 1156, 1192, 1254, 1367, 1391, 1433, 1444, 1479, 1584, 2864, 2902, 2977, 3051 cm^{-1}.

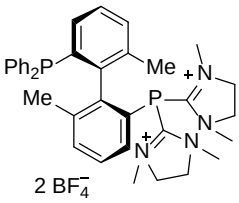


The previously prepared phosphate (600.0 mg, 1.194 mmol) in Et_2O (5 ml) was added to a suspension of $LiAlH_4$ (135.9 mg, 3.582 mmol) in Et_2O (5 ml) at -78 °C over the course of 30 min. The gray suspension obtained was stirred at -78 °C for additional 15 min and then allowed to warm to r.t. overnight. After this time, the reaction mixture was cooled to 0 °C

and deoxygenated water was carefully added until gas evolution ceased. The organic layer was then transferred into a schlenk and the remaining solid extracted with Et_2O (2 × 15 ml). Subsequently, the combined organic phases were dried with Na_2SO_4, filtered through Celite and the solvent removed *in vacuo* to afford *rac*-**5** as a white solid (404.1 mg, 85%).

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.43 (t, *J* = 6.8 Hz, 1H), 7.27 - 7.15 (m, 13H), 7.12 – 7.10 (m, 1H), 7.10 – 7.03 (m, 1H), 3.72 (dd, *J* = 31.6 Hz, *J* = 12.0 Hz, 1H), 3.21 (dd, *J* = 31.6 Hz; 12.0 Hz, 1H), 1.93 (s, 3H), 1.48 ppm (s, 3H); ^{13}C NMR ($CDCl_3$, 400 MHz): δ = 146.4 (dd, *J* = 31.4 Hz, *J* = 3.7 Hz), 144.1 (dd, *J* = 16.2 Hz, 7.0 Hz), 137.9 (d, *J* = 12.3 Hz), 137.5 (d, *J* = 9.8 Hz), 137.2 (t, *J* = 3.0 Hz), 136.7 (d, *J* = 12.3 Hz), 136.4 (d, *J* = 6.3 Hz), 134.6 (d, *J* = 21.1 Hz), 133.6 (d, *J* = 19.2 Hz), 132.5 (d, *J* = 9.8 Hz), 132.2 (d, *J* = 2.0 Hz), 131.1, 130.,0, 129.9 (d, *J* = 2.9 Hz), 128.8, 128.4 (d, *J* = 4.1 Hz), 128.36 (d, *J* = 2.7 Hz), 128.30, 127.9, 127.6 (d, *J* = 4.7 Hz), 20.1, 19.8 ppm; ^{31}P NMR ($CDCl_3$, 121 MHz): δ = -15.0 (d, $J_{P\text{-}P}$ = 20.1 Hz), -125.6 ppm (d, $J_{P\text{-}P}$ = 20.1 Hz); HRMS *calcd.* for $C_{26}H_{25}P_2^+$: 399.142680, *found* 399.142604; IR $\tilde{\nu}$ = 438, 490, 506, 537, 553, 573, 743, 768, 787, 827, 914, 998, 1026, 1067, 1094, 1147, 1206, 1261, 1306, 1379, 1400, 1434, 1475, 1566, 1584, 2294, 2851, 2913, 3001, 3048 cm^{-1}.

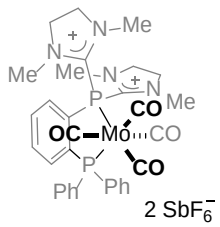
Compound **2:**



2-Chloro-1,3-dimethylimidazolidinium tetrafluoroborate **4** (110.0 mg, 0.502 mmol) and Et_3N (0.070 ml, 0.527 mmol) were added to a solution of *rac*-**5** (100.0 mg, 0.251 mmol) in THF (5 ml) and the resulting mixture stirred at 60 ^{o}C overnight. After cooling to r.t., the solvent was filtered off and the residue washed with $CHCl_3$, affording a white solid. Treatment with $NaBF_4$ (220.0 mg, 2.008 mmol) in CH_3CN (5 ml) and subsequent removal of the solvent *in vacuo* produced a white solid that was extracted with CH_2Cl_2 (3 × 10 ml). The combined organic phases were evaporated *in vacuo* affording *rac*-**2** as a white solid (78.9 mg, 41%). Colourless crystals suitable for X−ray crystallography were obtained from CH_3COCH_3/Et_2O solutions at r.t.

^{1}H NMR (CD_3CN, 400 MHz): δ = 7.71 – 7.70 (m, 1H), 7.56 – 7.50 (m, 2H), 7.47 – 7.26 (m, 10H), 7.16 – 7.09 (m, 3H), 4.07 (d, *J* = 2.4 Hz, 4H), 3.95 – 3.90 (m, 2H), 3.83 – 3.79 (m, 2H), 3.13 (s, 6H), 2.78 (s, *J* = 0.6 Hz, 6H), 1.81 (s, 3H), 1.20 ppm (m, 3H); ^{13}C NMR (CD_3CN, 100 MHz): δ = 166.1 (dd, *J* = 47.6 Hz; 0.8 Hz), 163.2 (dd, *J* = 53.2 Hz; 4.9 Hz), 145.7 (dd, *J* = 34.8 Hz; 5.7 Hz), 142.2 (dd, *J* = 8.2 Hz; 1.9 Hz), 141.5 (d, *J* = 7.2 Hz), 141.2 (d, *J* = 7.0 Hz), 140.0 (dd, *J* = 6.2 Hz; 1.4 Hz), 139.7 (dd, *J* = 34.8 Hz, *J* = 5.7 Hz), 137.1 (d, *J* = 8.9 Hz), 136.3 (d, *J* = 22.4 Hz), 135.9, 134.6, 133.8 (dd, *J* = 8.0 Hz; 3.9 Hz), 133.6 (d, *J* = 1.8 Hz), 133.4 (d, *J* = 3.4 Hz), 133.3 (d, *J* = 2.8 Hz), 132.8, 131.2, 131.1 (d, *J* = 0.9 Hz), 130.3 (d, *J* = 2.4 Hz), 129.9 (d, *J* = 5.9 Hz), 129.8 (d, *J* = 8.6 Hz), 54.5, 52.6, 38.0 (dd, *J* = 11.2 Hz; 3.5 Hz), 37.2 (d, *J* = 10.8 Hz), 19.5 (d, *J* = 2.3 Hz), 18.9 ppm (d, *J* = 3.2 Hz); ^{31}P NMR (CD_3CN, 121 MHz): δ = -14.6 (d, $J_{P\text{-}P}$ = 87.0 Hz), -44.3 ppm (d, $J_{P\text{-}P}$ = 87.0 Hz); ^{11}B NMR (CD_3CN, 96 MHz): δ = – 1.2 ppm; ^{19}F NMR (CD_3CN, 282 MHz): δ = –151.8 ppm; HRMS *calcd.* for $C_{36}H_{42}N_4BF_4P_2^+$: 679.290520; *found* 679.290843; IR $\tilde{\nu}$ = 438, 461, 480, 493, 506, 531, 576, 633, 646, 698, 746, 754, 767, 787, 931, 1024, 1047, 1223, 1297, 1332, 1363, 1411, 1435, 1447, 1526, 1579, 1709, 2923, 3504 cm^{-1}.

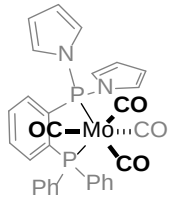
Compound **8:**



1a (36.4 mg, 0.038 mmol) and $Mo(CO)_6$ (10.0 mg, 0.038 mmol) were stirred in THF (2 ml) at 75 ^{o}C overnight. After cooling to r.t., the solvent was evaporated *in vacuo* and washed with CH_2Cl_2 to afford the desired compound as a yellow solid (19.9 mg, 49%). Yellow crystals suitable for X– ray analysis were obtained from a saturated solution in

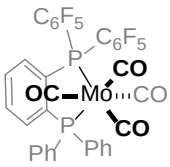
CH_3CN/Et_2O at r.t. ^{1}H NMR (CD_3CN, 400 MHz): δ = 8.15 – 8.07 (m, 1H), 8.04 – 7.89 (m, 3H), 7.68 – 7.27 (m, 10H), 4.01 (s, 8H), 3.14 – 2.92 (br, 12H). ^{13}C NMR (CD_3CN, 125 Mz): δ = 213.6 (dd, $J_{C–P}$ = 32.5, $J_{C–P}$ = 10.0 Hz), δ = 213.1 (dd, $J_{C–P}$ = 23.8, $J_{C–P}$ = 7.6 Hz), 208.2 (m), 162.4 (d, $J_{C–P}$ = 22.7Hz), 144.9 (dd, $J_{C–P}$ = 42.2, $J_{C–P}$ = 35.1 Hz), 138.4 (d, $J_{C–P}$ = 15.6 Hz), 136.5 (d, $J_{C–P}$ = 12.1 Hz), 136.2 (dd, $J_{C–P}$ = 4.7 Hz, $J_{C–P}$ = 2.2 Hz) , 135.1 (dd, $J_{C–P}$ = 5.8 Hz, $J_{C–P}$ = 1.7 Hz), 134.4 (d, $J_{C–P}$ = 13.2 Hz), 133.0 (m), 132.4, 130.3 (d, $J_{C–P}$ = 10.4 Hz), 129.8 (dd, $J_{C–P}$ = 41.6 Hz, 35.9 Hz), 53.5 (m), 53.5 ppm (m). ^{31}P NMR (CD_3CN, 162 MHz): δ = 60.1 (d, $J_{P–P}$ = 13.7 Hz), 40.2 ppm (d, $J_{P–P}$ = 13.7.7 Hz). ^{19}F NMR (CD_3CN, 282 MHz): δ = – 124.0 ppm (sextet, $J_{F–Sb(I=5/2)}$ = 1933 Hz, octet, $J_{F–Sb(I=7/2)}$ = 1049 Hz). HRMS *calcd.* for $C_{32}H_{34}N_4F_6MoP_2Sb^+$: 933.004530, *found* 933.004662. IR $\tilde{\nu}$ = 514, 524, 657, 697, 796, 1016, 1090, 1259, 1297, 1572, 1847, 1938, 1973, 2403, 2963 cm^{-1}.

Compound **9:**



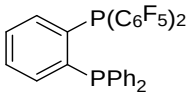
23 (100.0 mg, 0.236 mmol) and $Mo(CO)_6$ (62.2mg, 0.236 mmol) were stirred in THF (3 ml) overnight at 70 ^{o}C. After cooling to r.t., the solvent was evaporated *in vacuo* and crude **9** washed with diethylether. Yellow solid (113.2 mg, 76%). ^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 7.57 (m, 3H), 7.49 (m, 1H), 7.44 – 7.26 (m, 10H), 6.72 (dt, *J* = 4.2, *J* = 2.1 Hz, 4H), 6.32 ppm (td, *J* = 2.1, *J* = 1.1 Hz, 4H). ^{13}C NMR (CD_2Cl_2, 100 Mz): δ = 215.7 – 214.8 (m), 209.0 – 207.9 (m), 145.0 (dd, $J_{C–P}$ = 40.9, $J_{C–P}$ = 33.8 Hz), 143.1 (dd, $J_{C–P}$ = 42.9, $J_{C–P}$ = 34.9 Hz), 135.6 (dd, $J_{C–P}$ = 37.8, $J_{C–P}$ = 2.9 Hz), 133.9 (d, $J_{C–P}$ = 14.9 Hz), 132.6 (dd, $J_{C–P}$ = 5.0 Hz, $J_{C–P}$ = 2.0 Hz) , 132.6 (d, $J_{C–P}$ = 12.7 Hz), 131.1 (d, $J_{C–P}$ = 5.5 Hz), 130.6 (d, $J_{C–P}$ = 1.8 Hz), 130.5 (d, $J_{C–P}$ = 2.1 Hz), 129.0 (d, $J_{C–P}$ = 9.7 Hz), 124.3 (d, $J_{C–P}$ = 7.5 Hz), 113.0 ppm (d, $J_{C–P}$ = 5.7 Hz). ^{31}P NMR (CD_2Cl_2, 162 MHz): δ = 139.2 (d, $J_{P–P}$ = 4.7 Hz), 56.9 ppm (d, $J_{P–P}$ = 4.7 Hz). HRMS *calcd.* for $C_{30}H_{22}N_2O_4MoP_2Na^+$: 656.999890, *found* 657.000215. IR $\tilde{\nu}$ = 416, 504, 525, 571, 585, 671, 732, 999, 1037, 1067, 1116, 1177, 1234, 1434, 1449, 1481, 1572, 1896, 1936, 2030, 3062, 3251 cm^{-1}.

Compound **10:**



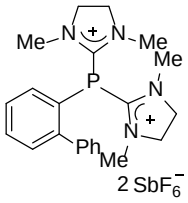
(Dipentafluorophenylphosphino)–2–diphenylphsphine **105** (100.0 mg, 0.160 mmol) and $Mo(CO)_6$ (42.2mg, 0.160 mmol) in THF (3 ml) was stirred at 70 ^{o}C overnight. After cooling to r.t., the solvent was evaporated *in vacuo* to afford the desired compound **107c** as a white solid (114.6 mg, 86%). ^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 7.76 – 7.72 (m, 1H), 7.61 – 7.56 (m, 4H), 7.43 – 7.40 ppm (m, 9H). ^{13}C NMR (CD_2Cl_2, 100 Mz): δ = 216.6 (dd, $J_{C–P}$ = 31.8, $J_{C–P}$ = 8.7 Hz), 215.1 (d, $J_{C–P}$ = 26.0 Hz), 208.5 (m), 146.5 (dm, $J_{C–F}$ = 251.0 Hz), 143.1 (dm, $J_{C–F}$ = 258.2 Hz), 142.9 (dd, $J_{C–P}$ = 43.4, $J_{C–P}$ = 35.0 Hz), 139.5 (m), 137.0 (m), 135.9 (dd, $J_{C–P}$ = 37.4, $J_{C–P}$ = 2.5 Hz), 134.8 (d, $J_{C–P}$ = 15.6 Hz), 133.4 (d, $J_{C–P}$ = 12.8 Hz), 132.5 (d, $J_{C–P}$ = 12.7 Hz), 131.7 (dd, $J_{C–P}$ = 16.5, $J_{C–P}$ = 2.0 Hz), 130.5 (d, *J* = 2.0 Hz), 128.9 (d, *J* = 9.7 Hz), 111.2 ppm (d, $J_{C–P}$ = 21.2 Hz). ^{31}P NMR (CD_2Cl_2, 162 MHz): δ = 60.5 (d, $J_{P–P}$ = 7.3 Hz), 31.1 ppm (q, $J_{P–F}$ = 10.6, $J_{P–F}$ = 10.1 Hz). ^{19}F NMR (CD_2Cl_2, 282 MHz): δ = – 128.6 (m), – 149.6 (m), – 160.0 ppm (m). EI–MS *calcd.* for $C_{34}H_{14}O_4F_{10}MoP_2$: 834.37, *found* 834.25. IR $\tilde{\nu}$ = 424, 542, 585, 631, 665, 693, 729, 799, 976, 1009, 1086, 1190, 1260, 1287, 1322, 1384, 1436, 1470, 1514, 1639, 1911, 2028, 2072, 2963, 3058 cm^{-1}.

Compound **12:**



^{n}BuLi (1.6 M in hexanes, 0.340 ml, 0.590 mmol) was added dropwise to (2–Bromophenyl)diphenylphosphine (200.0 mg, 0.586 mmol) in THF (5 ml) at – 78 °C and the mixture stirred for 1 h. at – 78 °C. $(C_6F_5)_2PCl$ (238.0 mg, 0.590 mmol) in THF (2 ml) was then added dropwise and the reaction mixture allowed to warm to r.t. overnight. After removal of all volatiles *in vacuo*, the crude was purified by column chromatography (SiO_2, hexane: toluene = 5: 1) to afford the desired diphosphine **12** as a white solid (103.5 mg, 28%). ^{1}H NMR (C_6D_6, 400 MHz): δ = 7.32 – 7.30 (m, 1H), 7.18 – 7.13 (m, 1H), 7.05 – 7.02 (m, 5H), 6.95 – 6.88 ppm (m, 7H). ^{13}C NMR (C_6D_6, 100 MHz): δ = 149.5 (m), 146.9 (m), 142.6 (dm, $J_{C–F}$ = 258.5 Hz), 138.3 (dd, J = 34.0 Hz, J = 11.4 Hz), 138.2 (d, J = 34.3 Hz, J = 11.4 Hz), 137.7 (q, $J_{C–F}$ = 252.8 Hz), 135.9 (q, J = 5.0 Hz), 133.7, 133.5, 132.7 (d, J = 8.9 Hz), 130.4, 129.8, 129.0, 128.8 ppm (d, J = 7.0 Hz). ^{31}P NMR (C_6D_6, 121 MHz): δ = – 16.6 (dt, $J_{P–F}$ = 184.5 Hz, $J_{P–P}$ = 5.1 Hz), – 56.4 ppm (dq, $J_{P–F}$ = 184.5 Hz, $J_{P–P}$ = 30.2 Hz). ^{19}F NMR (C_6D_6, 282 MHz): δ = – 129.2 (m), – 149.8 (m), – 160.5 ppm (m). HRMS *calcd.* for $C_{30}H_{14}F_{10}P_2$: 626.040937, *found* 626.041114. IR $\tilde{\nu}$ = 407, 439, 478, 494, 511, 521, 586, 631, 675, 745, 800, 840, 972, 1026, 1082, 1260, 1284, 1306, 1378, 1434, 1440, 1514, 1585, 1641, 2859, 2963, 3055 cm^{-1}.

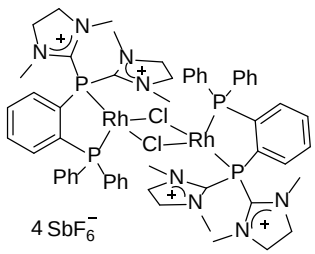
Compound **13:**



Et_3N (0.088 ml, 0.632 mmol) and **4** (132.6 mg, 0.602 mmol) were added to a solution of 2-(phenyl)phenylphoshine (56.0 mg, 0.30 mmol) in THF (5 ml) and the resulting mixture stirred at 60 °C overnight. After cooling to r.t., the solvent was filtered off affording a white powder that was dissolved in CH_2Cl_2 and washed twice with sat. $NaSbF_6$. The organic phase was dried and evaporation of the solvent afforded a white solid that was recrystallized from CH_3CN/Et_2O (60.9 mg, 24%).

^{1}H NMR (CD_3CN, 400 MHz): δ = 7.84 – 7.79 (m, 1H), 7.66 – 7.57 (m, 6H), 7.43 – 7.41 (m, 2H), 3.96 – 3.82 (m, 8H), 2.88 ppm (s, 12H); ^{13}C NMR (CD_3CN, 100 MHz): δ = 164.1 (d, J = 47.1 Hz), 150.1 (d, J = 34.1 Hz), 139.7 (d, J = 8.0 Hz), 135.7, 135.0, 133.0 (d, J = 6.0 Hz), 130.8 (d, J = 1.4 Hz), 130.5 (d, J = 13.8 Hz), 130.3 (d, J = 4.0 Hz), 128.9 (d, J = 24.1 Hz), 128.6, 53.4, 36.9 ppm (d, J = 9.0 Hz); ^{31}P NMR (CD_3CN, 121 MHz): δ = -43.1 ppm; ^{19}F NMR (CD_3CN, 282 MHz): δ = -124.0 ppm (sextet, $J_{F-123Sb}$ = 1945 Hz; octet, $J_{F-125Sb}$ = 1071 Hz); HRMS *calcd.* for $C_{22}H_{29}N_4F_6PSb^+$: 615.106410; *found* 615.106603; IR $\tilde{\nu}$ = 435, 455, 468, 554, 653, 707, 761, 779, 935, 1206, 1301, 1337, 1413, 1447, 1526, 1583 cm^{-1}.

Compound **14:**

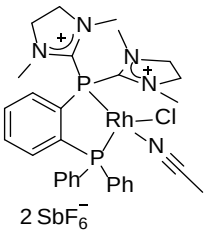


$[RhCl(cod)]_2$ (5.0 mg, 0.013 mmol) was added to a CH_2Cl_2 (2 ml) solution of **1a** (24.7 mg, 0.026 mmol) and the resulting mixture stirred overnight. After removal of the solvent *in vacuo*, the solid residue was washed with pentane, affording **14** as an orange solid (26 mg, 92%). Orange crystals of **14** suitable for X−ray crystallography were obtained by slow evaporation of solvent from a CH_2Cl_2 solution.

^{1}H NMR (CD_3CN, 400 MHz): δ = 7.94 – 7.7 (br, 16H), 7.57 – 7.47 (br, 12H), 3.95 (s, 16H), 3.17 ppm (s, 24H); ^{13}C NMR (CD_3CN, 100 MHz): δ = 156.9 (m), 136.1 (br), 135.9 (br), 135.7 (br), 135.0 (br), 132.5 (br), 129.7 (br), 53.4, 34.7 ppm; ^{31}P NMR (CD_3CN, 121 MHz): δ = 73.5 (dd, J_{P-Rh} = 151.7 Hz, J_{P-P} = 36.5 Hz,), 72.0 (br), 33.8 (br), 23.5 ppm (dd, J_{P-Rh} = 212.5 Hz, J_{P-P} = 36.5 Hz,); ^{19}F NMR (CD_3CN, 282 MHz): δ = -124.0 ppm

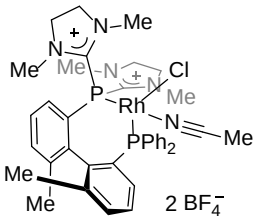
(sextet, $J_{F\text{-}121Sb}$ = 1945 Hz; octet, $J_{F\text{-}123Sb}$ = 1071 Hz); HRMS *calcd.* for $C_{56}H_{68}N_8Sb_3F_{18}P_4Cl_2Rh_2^+$: 1956.882960; *found* 1956.881010; IR $\tilde{\nu}$ = 491, 551, 616, 641, 678, 694, 747, 927, 1032, 1208, 1294, 1336, 1409, 1436, 1522, 1573, 2110, 2258, 2299, 2954 cm^{-1}.

Compound **15:**



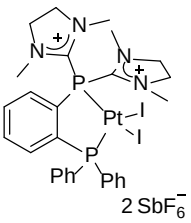
$[RhCl(COD)]_2$ (5.0 mg, 0.013 mmol) and **1a** (24.7 mg, 0.026 mmol) we dissolved in CH_2Cl_2 (2 ml) and stirred overnight. After removal of the solvent *in vacuo*, the solid obtained was washed with pentane affording the desired product **15** as an orange solid (26.3 mg, 92%). Orange crystals of **15** suitable for X−ray crystallography were directly obtained by cooling $CH_3CN/CH_2Cl_2/Et_2O$ solutions of the title compound. ^1H and ^{31}P NMR spectra of solutions of **15** in $CDCl_3$ showed a mixture of **14** and **15**, being **15** the major component.

Compound **16:**



$[RhCl(COD)]_2$ (6.4 mg, 0.013 mmol) and **2** (20.0 mg, 0.026 mmol) were dissolved in CH_3CN (2 m l) and stirred overnight. After removal of the solvent *in vacuo*, the solid obtained washed with CH_2Cl_2 and pentane, and subsequently dried, affording **16** as a yellow solid (21.6 mg, 86%). Yellow crystals suitable for X−ray crystallography were obtained from a saturated $CH_3CN/CH_2Cl_2/Et_2O$ solution at r.t. ^1H NMR (CD_3CN, 400 MHz): δ = 7.75 – 8.60 (m, 3H), 7.59 – 7.42 (m, 7H), 7.42 – 7.35 (m, 3H), 7.33 – 7.28 (m, 1H), 7.26 – 7.16 (m, 1H), 7.14 – 7.10 (m, 1H), 4.32 – 4.20 (m, 2H), 4.16 (s, 3H), 4.02 (s, 3H), 3.96 – 3.90 (m, 2H), 3.81 – 3.89 (m, 1H), 3.78 – 3.66 (m, 2H), 3.45 – 3.33 (m, 1H), 3.03 (s, 3H), 2.75 (s, 3H), 1.74 (s, 3H), 1.62 ppm (s, 3H). ^{13}C NMR (CD_3CN, 125 MHz): δ = 164.8 (d, *J* = 33.6 Hz), 154.8, 143.1 (d, *J* = 9.5 Hz), 142.5 (d, *J* = 7.6 Hz), 140.5 (d, *J* = 18.2 Hz, *J* = 4.0 Hz), 137.0 (d, *J* = 52.9 Hz), 136.9 (dd, *J* = 11.5 Hz, *J* = 6.1 Hz), 135.9, 135.7 (d, J_{C-P} = 10.4 Hz), 135.5 (d, *J* = 12.9 Hz), 134.8, 132.7, 132.3 (d, *J* = 50.0 Hz), 132.0, 131.2 (d, *J* = 7.6 Hz), 130.1 (d, *J* = 9.3 Hz), 130.0 (d, *J* = 5.3 Hz), 129.6 (d, *J* = 10.6 Hz), 129.5 (d, *J* = 10.0 Hz), 129.4 (d, *J* = 9.7 Hz), 127.8 (d, *J* = 51.0 Hz), 121.7 (d, *J* = 59.1 Hz), 55.4, 53.7, 53.6, 51.5, 42.6 (d, *J* = 4.4 Hz), 39.4 (d, *J* = 11.0 Hz), 39.0, 37.4, 20.7, 19.8 ppm. ^{31}P NMR (CD_3CN, 121 MHz): δ = 38.1 (dd, J_{P-Rh} = 153.9 Hz, J_{P-P} = 50.2 Hz), 11.9 ppm (dd, J_{P-Rh} = 215.7 Hz, J_{P-P} = 50.2 Hz). ^{11}B NMR (CD_3CN, 96 MHz): δ = – 1.2 ppm, ^{19}F NMR (CD_3CN, 282 MHz): δ = – 151.9 ppm. IR $\tilde{\nu}$ = 463, 698, 754, 792, 868, 936, 1052, 1292, 1401, 1661, 2112, 2325, 3205, 3369 cm^{-1}.

Compound **17:**



CH_2Cl_2 (2 ml) was added to a mixture of $PtI_2(PhCN)_2$ (20.0 mg, 0.031 mmol) and **1a** (29.5 mg, 0.031 mmol) and the resulting solution stirred overnight. After removal of the solvent *in vacuo*, the solid residue was washed with pentane, affording **17** as a yellow solid (40.3 mg, 95%). Yellow crystals suitable for X−ray crystallography were obtained from CH_3COCH_3/Et_2O at 0 °C.

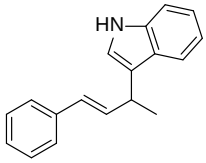
^1H NMR (CD_3CN, 400 MHz): δ = 8.45 – 8.40 (m, 1H), 7.96 – 7.91 (m, 2H), 7.77 – 7.70 (m, 7H), 7.62 – 7.57 (m, 4H), 4.07 – 4.00 (m, 8H), 3.24 ppm (s, 12H); ^{13}C NMR (CD_3CN, 100 MHz): δ = 154.3 (d, *J*

= 49.5 Hz), 138.7 (m), 136.3 (m), 136.2 (m), 136.1 (m), 135.9 (m), 135.1 (dd, 19.4 Hz; 8.1 Hz), 134.5 (d, J = 3.6 Hz), 130.5(d, J = 12.3 Hz), 127.6 (d, J = 68.7 Hz), 54.5 (d, J = 3.3 Hz), 39.6 (d, J = 3.0 Hz) ppm; ^{31}P NMR (CD_3CN, 121 MHz): δ = 39.2 (dt, $J_{P\text{-}P}$ = 4.6 Hz, $J_{P\text{-}Pt}$ = 1429 Hz), 5.4 ppm (dt, $J_{P\text{-}P}$ = 4.6 Hz, $J_{P\text{-}Pt}$ = 1723 Hz); ^{19}F NMR (CD_3CN, 282 MHz): δ = -124.0 ppm (sextet, $J_{F\text{-}121Sb}$ = 1945 Hz, octet, $J_{F\text{-}123Sb}$ = 1071 Hz); HRMS *calcd.* for $C_{28}H_{34}N_4SbF_6P_2I_2Pt^+$: 1171.893620; *found* 1171.893250; IR $\tilde{\nu}$ = 452, 503, 543, 598, 645, 689, 750, 922, 998, 1101, 1114, 1300, 1408, 1437, 1520, 1586, 1979, 2220, 3007, 3061 cm^{-1}.

General procedure for the synthesis of compounds **19a-m**:

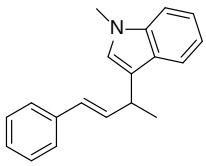
Phenyl-1,3–butadiene (26.0 mg, 0.200 mmol) and the desired nucleophile (0.220 mmol, 1.1 eq) were added to a preformed solution containing **1a** (9.6 mg, 0.010 mmol), $[RhCl(CO)_2]_2$ (1.9 mg, 0.005 mmol) and $KB(Ar^F)_4$ (14.3 mg, 0.020) in DCE (1 ml). The solution thus obtained was stirred at 70 °C for 12-18 h. Once finished, the solvents were evaporated and the resulting oil purified by column chromatography (SiO_2, Hexane:EtOAc = 20:1) to afford the desired hydroarylation product **19a-m.**

Compound **19a:**



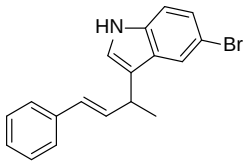
Colorless oil (41.0 mg, 86% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.95 (br, 1H), 7.69 (dd, J = 7.9 Hz, J = 0.6 Hz, 1H), 7.40 – 7.35 (m, 3H), 7.31 – 7.27 (m, 2H), 7.23 – 7.17 (m, 2H), 7.10 (ddd, J = 7.9 Hz, J = 7.8 Hz, J = 0.6 Hz, 1H), 7.03 (dd, J = 2.3 Hz, J = 0.6 Hz, 1H), 6.51 – 6.48 (m, 2H), 3.95 (p, J = 6.8 Hz, 1H), 1.58 ppm (d, J = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 137.9, 136.7, 135.6, 128.6, 128.3, 127.0, 126.9, 126.3, 122.1, 120.6, 120.5, 119.8, 119.4, 111.2, 34.4, 20.8 ppm. HRMS *calcd.* for $C_{18}H_{18}N^+$: 248.143420, *found* 248.143374. IR $\tilde{\nu}$ = 424, 497, 581, 693, 742, 765, 807, 928, 966, 1009, 1095, 1221, 1244, 1337, 1417, 1455, 1492, 1598, 1618, 2869, 2927, 2963, 3024, 3055, 3417 cm^{-1}.

Compound **19b**



Colorless oil (32.1 mg, 63% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.67 (dm, J = 7.9 Hz, 1H), 7.38 – 7.25 (m, 2H), 7.31 – 7.27 (m, 2H), 7.24 – 7.21 (m, 1H), 7.21 – 7.16 (m, 1H), 7.01 – 7.06 (m, 1H), 6.88 (s, 1H), 6.54 – 6.43 (m, 2H), 3.93 (p, J = 6.8 Hz, 1H), 3.76 (s, 3H), 1.56 ppm (d, J = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 137.9, 137.4, 135.7, 128.6, 128.1, 127.3, 127.0, 126.3, 125.4, 121.7, 119.8, 119.0, 118.8, 109.3, 34.3, 32.8, 21.0 ppm. HRMS *calcd.* for $C_{19}H_{19}NNa^+$: 284.141100, *found* 284.140968. IR $\tilde{\nu}$ = 424, 497, 581, 698, 746, 968, 992, 1093, 1242, 1373, 1470, 1493, 1528, 1613, 1712, 1778, 2930, 2961, 3026, 3055 cm^{-1}.

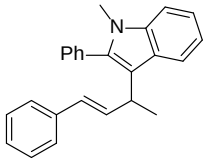
Compound **19c:**



Yellow oil (53.5 mg, 82% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.00 (br, 1H), 7.78 (m, 1H), 7.40 – 7.35 (m, 2H), 7.31 – 7.28 (m, 2H), 7.27 – 7.25 (m, 2H), 7.23 – 7.17 (m, 2H), 7.03 (d, J = 2.0 Hz, 1H), 6.51 – 6.39 (m, 1H), 3.88 (p, J = 6.7 Hz, 1H), 1.55 ppm

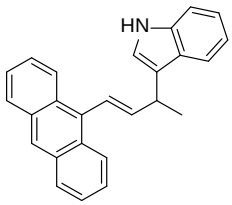
(d, J = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 137.7, 135.3, 135.0, 128.7, 128.6, 128.6, 127.1, 126.3, 125.0, 122.3, 121.8, 120.4, 112.7, 34.2, 20.9 ppm. HRMS *calcd.* for $C_{18}H_{15}NBr^+$: 324.039610, *found* 324.039349. IR ϋ = 421, 488, 583, 696, 749, 795, 865, 996, 1045, 1096, 1260, 1373, 1458, 1493, 1599, 1721, 2927, 2962, 3025, 3421 cm^{-1}.

Compound **19d:**



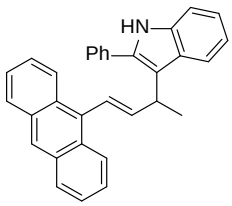
Colorless oil (52.1 mg, 76% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.76 (dm, J = 8.0 Hz, 1H), 7.53 – 7.45 (m, 3H), 7.44 – 7.40 (m, 2H), 7.37 (dm, J = 8.0 Hz, 1H), 7.34 – 7.30 (m, 2H), 7.28 (m, 3H), 7.17 (tm, J = 7.1 Hz, 1H), 7.11 (tm, J = 7.4 Hz, 1H), 6.62 (dd, J = 15.9 Hz, J = 5.8 Hz, 1H), 6.39 (dd, J = 15.9 Hz, J = 1.5 Hz, 1H), 3.80 (m, 1H), 3.58 (s, 3H), 1.56 ppm (d, J = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 138.1, 137.5, 135.7, 132.3, 131.0, 128.6, 128.5, 128.4, 128.3, 128.0, 126.9, 126.4, 126.2, 121.6, 120.7, 119.2, 116.3, 116.2, 109.6, 34.4, 30.9, 21.1 ppm. HRMS *calcd.* for $C_{25}H_{23}NNa^+$: 360.172400, *found* 360.172268. IR $\tilde{\nu}$ = 435, 486, 520, 592, 582, 601, 722, 735, 805, 921, 964, 1017, 1098, 1135, 1157, 1247, 1264, 1335, 1362, 1397, 1429, 1466, 1492, 1600, 2926, 2963, 3025 cm^{-1}.

Compound **19e:**



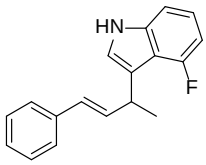
Pale yellow solid (66.0 mg, 95% yield). ^{1}H NMR (600 MHz, C_6D_6) δ 8.44 – 8.40 (m, 2H), 8.15 (s, 1H), 7.93 – 7.89 (m, 1H), 7.83 – 7.80 (m, 2H), 7.29 – 7.24 (m, 6H), 7.11 – 7.08 (m, 2H), 6.62 (s, 1H), 6.53 (d, J = 2.4 Hz, 1H), 6.21 (dd, J = 16.1, 7.0 Hz, 1H), 4.05 – 3.99 (m, 1H), 1.58 (d, J = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, C_6D_6) δ 143.97, 132.06, 130.30, 128.89, 126.67, 126.36, 125.34, 125.23, 124.46, 122.30, 120.43, 120.10, 119.60, 111.49. HRMS *calcd.* for $C_{26}H_{21}N^+$: 347.1674, *found* 347.1667. IR $\tilde{\nu}$ = 668, 737, 1012, 1338, 1351, 1417, 1456, 1488, 1621, 1654, 1670, 1683, 1698, 2341, 2360, 2869, 2926, 2964, 3049, 3421, 3627, 3733 cm^{-1}.

Compound **19f:**



Yellow solid (57.6 mg, 68% yield). ^{1}H NMR (400 MHz, C_6D_6) δ 8.38 – 8.32 (m, 2H), 8.09 (s, 1H), 8.00 – 7.95 (m, 1H), 7.79 – 7.73 (m, 2H), 7.42 – 7.36 (m, 2H), 7.31 – 7.15 (m, 8H), 6.99 – 6.90 (m, 2H), 6.41 (dd, J = 16.2, 5.3 Hz, 1H), 4.33 (tdd, J = 7.3, 5.3, 1.9 Hz, 1H), 1.63 (d, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, C_6D_6) δ 159.66, 157.97, 143.66, 133.91, 131.77, 130.02, 128.58, 126.38, 126.16, 125.98, 124.99, 124.91, 123.88, 104.18, 98.96, 54.56, 54.54, 36.14, 20.19. HRMS *calcd.* for $C_{32}H_{25}NNa^+$: 446.1885, *found* 446.1865. IR $\tilde{\nu}$ = 689, 698, 738, 764, 798, 1002, 1024, 1259, 1284, 1311, 1449, 1579, 1600, 1672, 1760, 2357, 2923, 2963cm^{-1}.

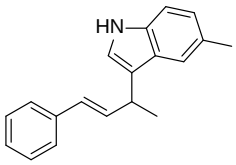
Compound **19g:**



Light yellow oil (34.4 mg, 65% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.00 (br, 1H), 7.36 – 7.33 (m, 2H), 7.28 – 7.25 (m, 2H), 7.18 – 7.17 (m, 1H), 7.14 – 7.11 (m, 1H), 7.09 – 7.05 (m, 1H), 6.96 – 6.95 (m, 1H), 6.76 – 71 (m, 1H), 6.54 – 6.42 (m, 2H), 4.08 (p, J = 6.8 Hz,

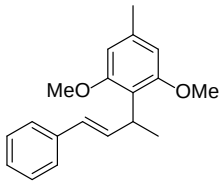
1H), 1.53 ppm (d, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 152.3 (d, *J* = 247.0 Hz), 139.4 (d, *J* = 11.9), 138.1, 135.6 (d, *J* = 0.8), 128.6, 128.4 (d, *J* = 7.6), 128.2 (d, *J* = 1.0), 127.0, 126.3, 125.8 (d, *J* = 35.1), 122.7 (d, *J* = 8.0), 120.5 (d, *J* = 1.3), 120.3 (d, *J* = 3.9 Hz), 115.7 (d, *J* = 20.2), 115.7 (d, *J* = 20.2), 107.3 (d, *J* = 3.6), 104.9 (d, *J* = 20.2), 34.8 (d, *J* = 1.4), 21.5 ppm (d, *J* = 1.9). ^{19}F NMR ($CDCl_3$, 282 MHz): δ = – 120.8 ppm. HRMS *calcd.* for $C_{18}H_{15}NF^+$: 264.119600, *found* 264.119402. IR $\tilde{\nu}$ = 483, 649, 696, 732, 780, 908, 996, 1035, 1224, 1348, 1446, 1494, 1578, 1628, 1628, 1694, 2962, 3025, 3416 cm^{-1}.

Compound **19h**



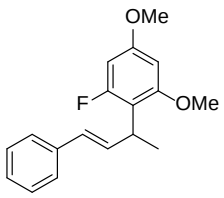
5–Methylindol (28.9 mg, 0.220 mmol) and phenyl 1,3–butadiene (26.0 mg, 0.200 mmol) were added to a solution of **92b** (9.6 mg, 0.010 mmol), $[RhCl(CO)_2]_2$ (1.9 mg, 0.005 mmol) and $KB(Ar^F)_4$ (14.3 mg, 0.020) in DCE (1 ml), and the reaction mixture was stirred at 70 °C for 18 h. The resulting oil was purified by column chromatography (SiO_2, Hexane:EtOAc = 100:1 to 20:1) to afford the desired compound **121** as a light yellow oil (41.2 mg, 76% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.86 (br, 1H), 7.45 (m, 1H), 7.38 – 7.35 (m, 2H), 7.30 – 7.25 (m, 3H), 7.19 (tm, *J* = 8.4 Hz, 1H), 7.2 (dd, *J* = 8.3 Hz, *J* = 1.2 Hz, 1H), 7.00 (d, *J* = 2.3 Hz, 1H), 6.49 – 6.43 (m, 2H), 3.95 – 3.88 (m, 1H), 2.44 (s, 3H), 1.56 ppm (d, *J* = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 138.0, 135.7, 135.0, 128.6, 128.2, 127.1, 127.0, 126.3, 126.9, 123.7, 120.7, 120.1, 119.3, 110.9, 34.3, 21.7, 20.9 ppm. HRMS *calcd.* for $C_{19}H_{19}NNa^+$: 284.141150, *found* 284.140968. IR $\tilde{\nu}$ = 423, 460, 493, 589, 696, 748, 793, 698, 920, 996, 1012, 1029, 1073, 1096, 1182, 1224, 1320, 1369, 1419, 1448, 1493, 1580, 1598, 2867, 2925, 2962, 3023, 3414 cm^{-1}.

Compound **19i:**



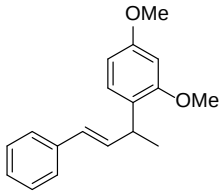
Colorless oil (48.0 mg, 85% yield). ^{1}H NMR (300 MHz, Chloroform-d) δ 7.38 – 7.33 (m, 2H), 7.31 – 7.24 (m, 3H), 7.23 – 7.13 (m, 1H), 6.71 (dd, *J* = 15.9, 7.4 Hz, 1H), 4.29 (td, *J* = 7.2, 1.3 Hz, 1H), 3.83 (s, 6H), 2.35 (s, 3H), 1.45 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.05, 138.48, 137.13, 135.59, 128.28, 127.56, 126.39, 126.00, 119.07, 105.55, 55.85, 32.71, 21.88, 19.22. HRMS *calcd.* for $C_{19}H_{23}O_2^+$: 283.1693, *found* 283.1693. IR $\tilde{\nu}$ = 669, 801, 882, 943, 963, 1008, 1027, 1167, 1253, 1453, 2341, 2360, 2872, 2927, 2966, 3024 cm^{-1}.

Compound **19j** (major regioisomer)**:**



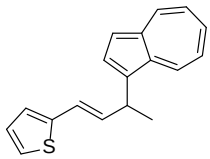
Colorless oil (39.0 mg, 82% yield). ^{1}H NMR (400 MHz, Chloroform-d) δ 7.35 – 7.30 (m, 2H), 7.28 – 7.21 (m, 3H), 7.18 – 7.11 (m, 1H), 6.54 (ddd, *J* = 15.9, 7.3, 2.1 Hz, 1H), 6.36 (d, *J* = 15.9 Hz, 1H), 6.27 – 6.18 (m, 2H), 4.13 – 4.04 (m, 1H), 3.82 (s, 1H), 3.80 (s, 2H), 3.75 (s, 3H), 1.46 – 1.37 (m, 3H). ^{19}F NMR (282 MHz, Chloroform-d) δ -100.01. ^{13}C NMR (101 MHz, C_6D_6) δ 163.67, 161.27, 159.74, 159.60, 158.89, 158.77, 156.79, 138.05, 138.03, 134.11, 134.01, 133.99, 128.80, 128.32, 126.71, 126.26, 95.24, 95.21, 93.51, 93.23, 55.13, 54.95, 54.61, 32.73, 19.67, 19.64. HRMS *calcd.* for $C_{18}H_{19}FO_2^+$: 286.1369, *found* 286.1372. IR $\tilde{\nu}$ = 745, 803, 820, 964, 1017, 1053, 1198, 1213, 1422, 1438, 1454, 1493, 1584, 1620, 2360, 2934, 2961 cm^{-1}.

Compound **19k:**



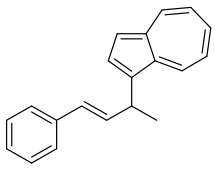
Colorless oil (37.8 mg, 71% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.37 – 7.34 (m, 2H), 7.30 – 7.27 (m, 2H), 7.20 – 7.15 (m, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 6.47 – 6.40 (m, 4H), 4.00 – 3.97 (m, 1H), 3.83 (s, 3H), 3.80 (s, 3H), 1.39 ppm (d, *J* = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 159.3, 157.9, 138.1, 135.4, 128.6, 128.1, 128.0, 126.9, 126.7, 126.2, 104.3, 98.9, 55.6, 55.5, 34.8, 20.3 ppm. HRMS *calcd.* for $C_{18}H_{21}O_2^+$: 269.153580, *found* 269.135605. IR $\tilde{\nu}$ = 495, 634, 692, 737, 798, 909, 966, 1034, 1117, 1156, 1179, 1206, 1259, 1290, 1417, 1453, 1503, 1586, 1610, 2835, 2928, 2959, 3024 cm^{-1}.

Compound **19l:**



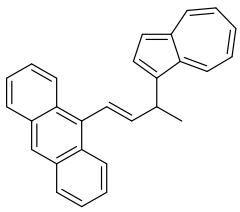
Blue oil (48.8 mg, 68% yield). ^{1}H NMR (400 MHz, Chloroform-d) δ 8.41 – 8.22 (m, 2H), 7.86 (d, *J* = 3.8 Hz, 1H), 7.64 – 7.47 (m, 1H), 7.37 (d, *J* = 3.9 Hz, 1H), 7.15 – 7.04 (m, 3H), 6.96 – 6.75 (m, 1H), 6.53 – 6.30 (m, 2H), 4.30 (p, *J* = 6.8 Hz, 1H), 1.61 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.02, 140.85, 137.47, 136.65, 135.91, 135.24, 134.99, 133.36, 133.26, 127.19, 124.59, 123.26, 122.39, 121.74, 121.36, 116.98, 34.80, 21.72. HRMS *calcd.* for $C_{18}H_{16}SNa^+$: 287.0870, *found* 287.0861. IR $\tilde{\nu}$ = 759.8, 1026.9, 1053.9, 1065.5, 1075.1, 1260.3, 1394.3, 2341.2, 2360.4, 2900.4, 2966.9, 2987.2 cm^{-1}.

Compound **19m:**



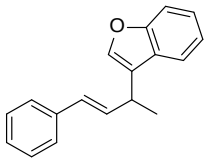
Blue solid (36.5 mg, 72% yield). ^{1}H NMR (400 MHz, Chloroform-d) δ 8.37 (d, *J* = 9.7 Hz, 1H), 8.27 (dd, *J* = 9.4, 1.0 Hz, 1H), 7.87 (d, *J* = 3.9 Hz, 1H), 7.58 – 7.49 (m, 1H), 7.38 – 7.29 (m, 3H), 7.19 – 7.04 (m, 3H), 6.51 (dd, *J* = 15.9, 6.4 Hz, 1H), 6.39 (dd, *J* = 15.8, 1.2 Hz, 1H), 4.38 – 4.25 (m, 1H), 1.63 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 140.84, 137.74, 137.44, 136.62, 135.98, 135.14, 134.97, 133.76, 133.30, 128.43, 127.85, 126.88, 126.11, 122.33, 121.67, 116.94, 35.05, 21.82. HRMS *calcd.* for $C_{20}H_{18}^+$: 258.1409, *found* 258.1411. IR $\tilde{\nu}$ =529, 577, 671, 712, 771, 846, 870, 893, 943, 961, 1015, 1028, 1198, 1296, 1370, 1392, 1412, 1430, 1447, 1493, 1533, 1574, 2925, 2959, 3021 cm^{-1}.

Compound **19n:**



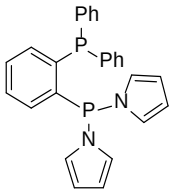
Blue solid (48.8 mg, 68% yield). ^{1}H NMR (400 MHz, Benzene-d6) δ 8.31 (ddd, *J* = 7.7, 3.9, 1.9 Hz, 3H), 8.10 (s, 1H), 7.96 (d, *J* = 9.3 Hz, 1H), 7.88 (d, *J* = 3.9 Hz, 1H), 7.79 – 7.75 (m, 2H), 7.31 (d, *J* = 4.0 Hz, 1H), 7.24 – 7.17 (m, 5H), 6.96 (dt, *J* = 16.2, 1.2 Hz, 1H), 6.84 (t, *J* = 9.8 Hz, 1H), 6.72 (t, *J* = 9.6 Hz, 1H), 6.18 (dd, *J* = 16.1, 6.6 Hz, 1H), 4.34 – 4.25 (m, 1H), 1.59 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, C6D6) δ 144.21, 137.07, 136.55, 135.23, 133.21, 131.72, 129.94, 128.59, 126.22, 126.07, 125.04, 124.91, 123.81, 122.15, 121.37, 117.47, 35.77, 21.76. HRMS *calcd.* for $C_{28}H_{22}^+$: 358.1721, *found* 358.1716. IR $\tilde{\nu}$ = 543, 720, 773, 784, 800, 845, 887, 973, 1015, 1046, 1260, 1394, 1448, 1575, 2360, 2851, 2922, cm^{-1}.

Compound **19o:**



Yellow oil (15.4 mg, 31% yield) ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.53 – 7.49 (m, 1H), 7.44 – 7.36 (m, 4H), 7.33 – 7.27 (m, 3H), 7.24 – 7.15 (m, 4H), 6.57 – 6.48 (m, 2H), 6.39 (dd, *J* = 16.0, 7.3 Hz, 1H), 3.84 (tt, *J* = 7.1, 1.1 Hz, 1H), 3.43 (q, *J* = 7.0 Hz, 1H), 1.55 (d, *J* = 7.0 Hz, 3H), 1.15 (t, *J* = 7.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.84, 137.74, 137.44, 136.62, 135.98, 135.14, 134.97, 133.76, 133.30, 128.43, 127.85, 126.88, 126.11, 122.33, 121.67, 116.94, 35.05, 21.82. HRMS *calcd.* for $C_{25}H_{23}NNa^{+}$: 360.172400, *found* 360.172268. IR $\tilde{\nu}$ = 435, 486, 520, 592, 582, 601, 722, 735, 805, 921, 964, 1017, 1098, 1135, 1157, 1247, 1264, 1335, 1362, 1397, 1429, 1466, 1492, 1600, 2926, 2963, 3025 cm^{-1}.

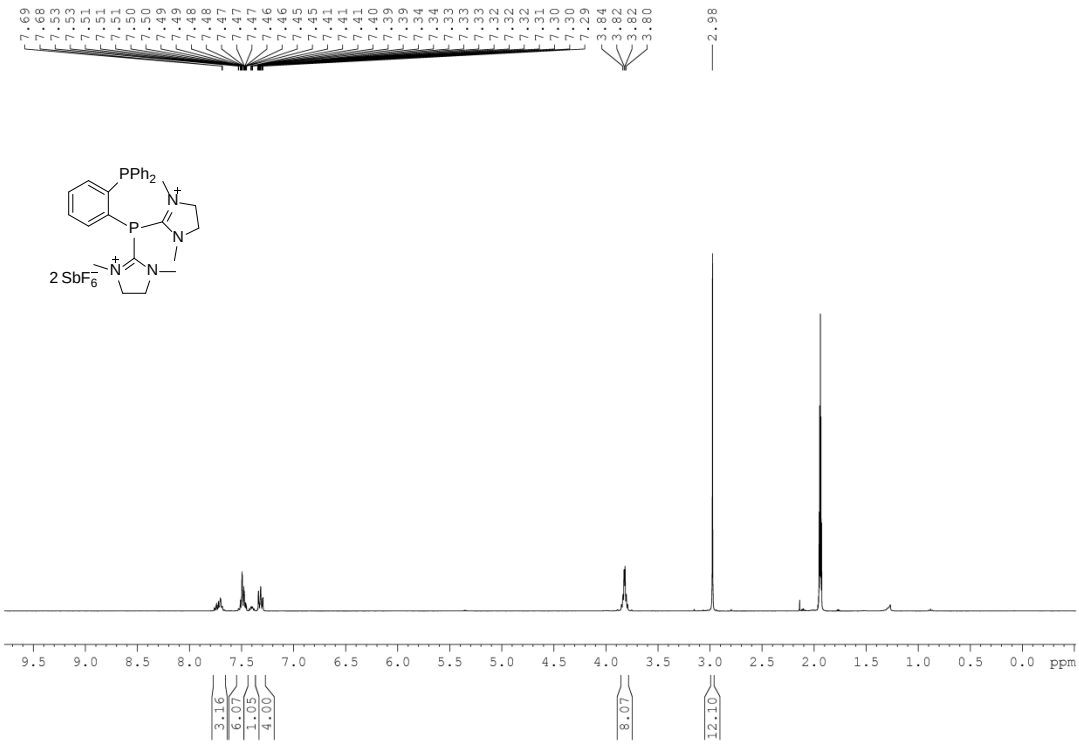
Compound **20:**



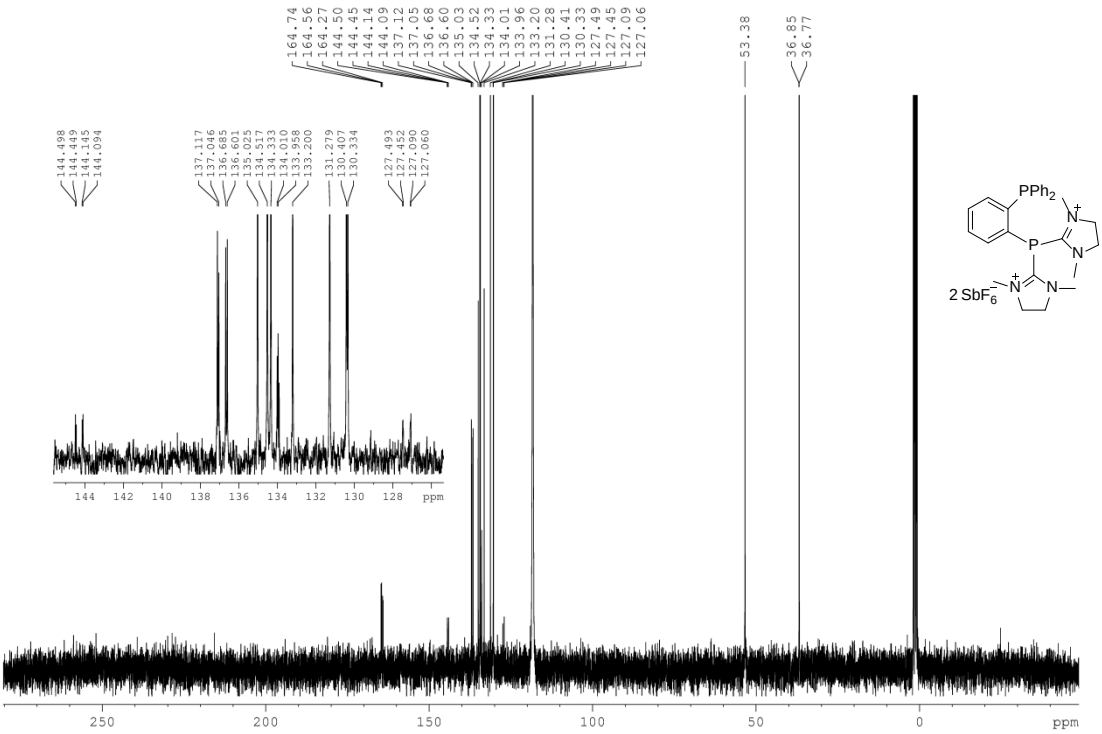
^{n}BuLi (1.6 M in hexanes, 0.689 ml, 1.102 mmol) was added dropwise to (2–bromophenyl)diphenylphosphine (376.0 mg, 1.102 mmol) in THF (5 ml) at – 78 °C. The mixture was stirred for 1 h at – 78 °C and then a THF solution of (pyrrolyl)$_2$PCl (218.9 mg, 1.102 mmol) THF (2 ml) was added dropwise. The reaction was then allowed to warm to r.t. overnight before all volatiles were removed *in vacuo*. Crude 21 thus obtained was purified by column chromatography (SiO_2, hexane:toluene = 3:1). White solid (304.2 mg, 65%). ^{1}H NMR (C_6D_6, 300 MHz): δ = 7.29 – 7.26 (m, 1H), 7.21 – 7.19 (m, 3H), 7.00 – 7.97 (m, 7H), 6.92 – 6.88 (m, 2H), 6.81 – 6.78 (m, 1H), 6.76 – 6.74 (m, 4H), 6.23 ppm (t, *J* = 2.1Hz, 4H). ^{13}C NMR (C_6D_6, 100 Mz): δ = 144.6 (dd, $J_{C–P}$ = 32.3, $J_{C–P}$ = 12.6 Hz), 141.9 (dd, $J_{C–P}$ = 28.3, $J_{C–P}$ = 14.2 Hz), 136.5 (dd, $J_{C–P}$ = 10.3, $J_{C–P}$ = 4.6 Hz), 135.5 (d, $J_{C–P}$ = 3.2 Hz), 133.8 (d, $J_{C–P}$ = 19.6 Hz), 130.6 (dd, $J_{C–P}$ = 10.3, 5.3 Hz), 130.5 (d, $J_{C–P}$ = 73.1 Hz), 128.8, 128.7 (d, $J_{C–P}$ = 7.0 Hz), 127.3, 124.6 (d, $J_{C–P}$ = 13.8 Hz), 112.6 ppm (d, $J_{C–P}$ = 3.9 Hz). ^{31}P NMR (C_6D_6, 121 MHz): δ = 66.1 (d, $J_{P–P}$ = 167.3 Hz), – 18.6 ppm (d, $J_{P–P}$ = 167.3 Hz). HRMS *calcd.* for $C_{26}H_{22}N_2P_2Na^{+}$: 447.114760, *found* 447.115045. IR $\tilde{\nu}$ = 419, 474, 498, 546, 616, 662, 693, 731, 766, 803, 100, 1057, 1074, 1176, 1241, 1262, 1292, 1389, 1434, 1449, 1478, 1555, 1582, 2924, 2961, 3063 cm^{-1}.

Selected NMR Spectra:

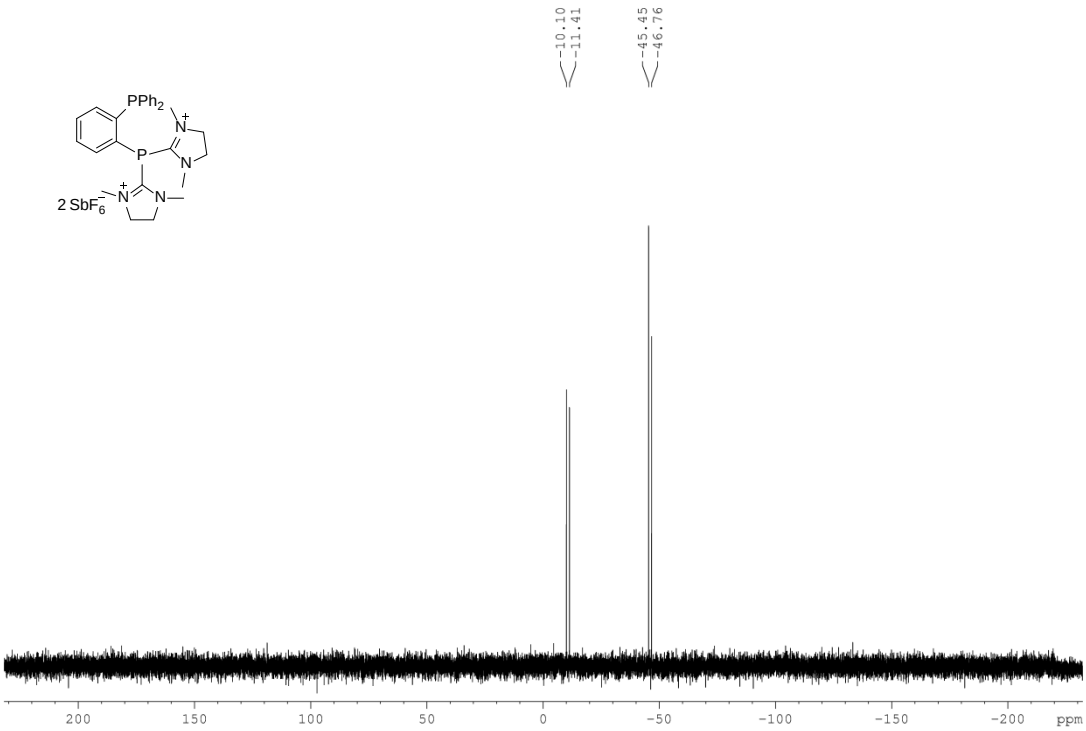
^{1}H-NMR (CD_3CN, 400 MHz) of **1a**:



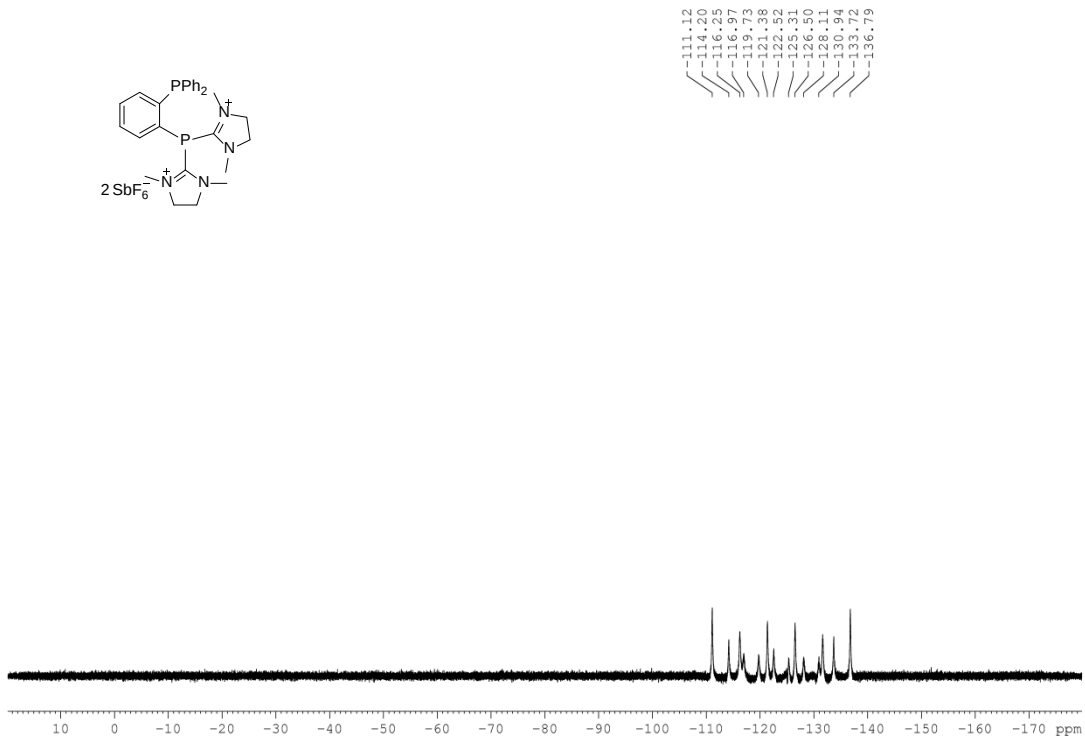
^{13}C NMR (CD_3CN, 100 MHz) of **1a**:



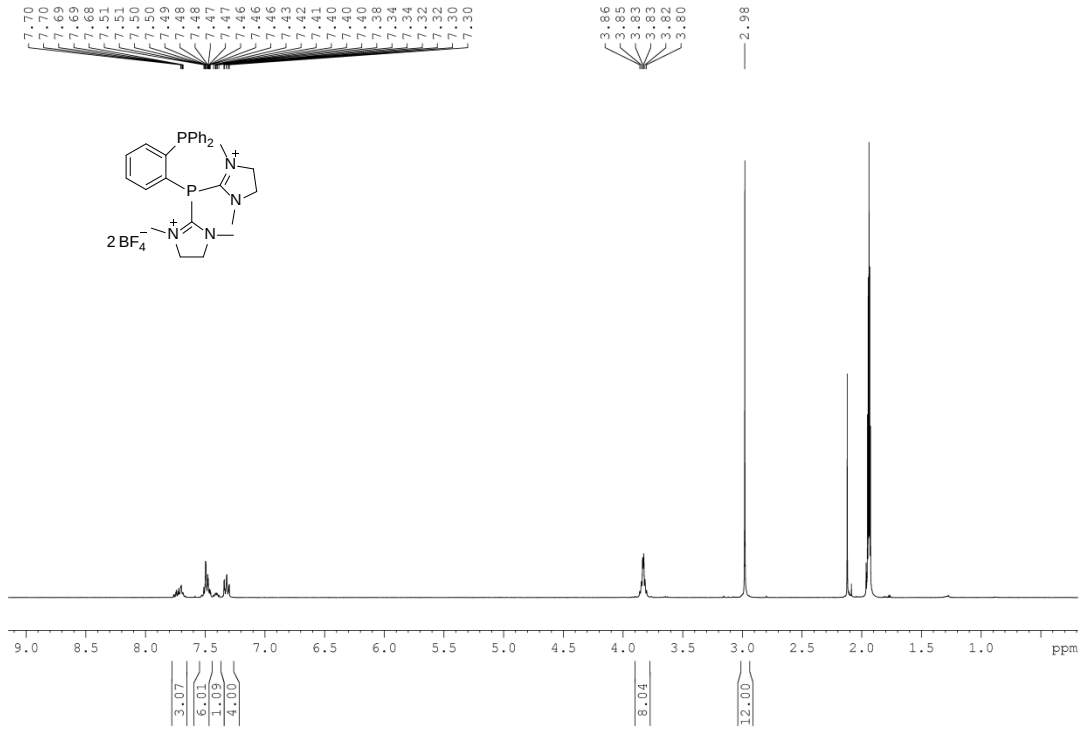
^{31}P NMR (CD_3CN, 121 MHz) of **1a**:



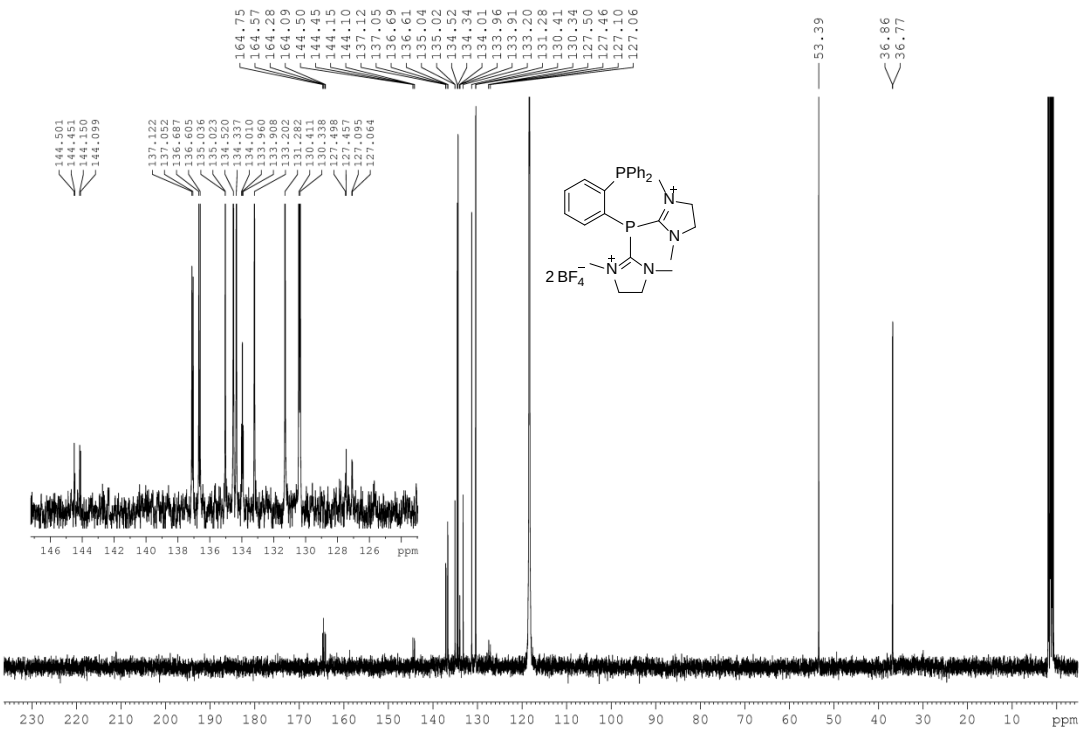
^{19}F NMR (CD_3CN, 376 MHz) of **1a**:



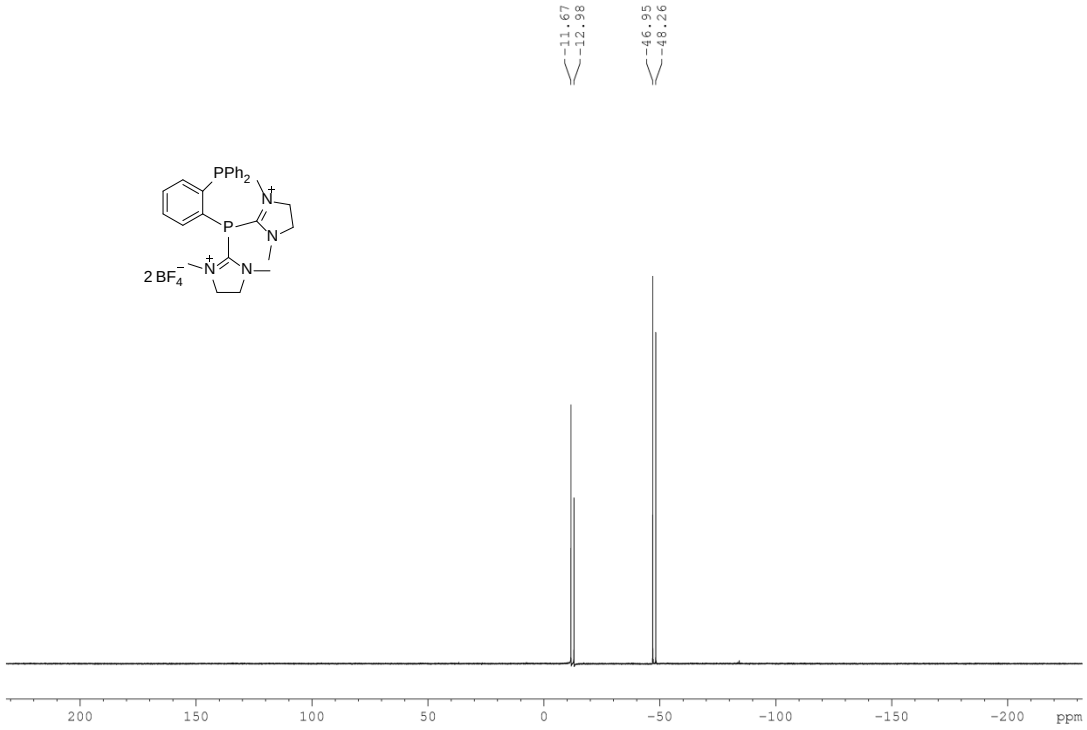
^{1}H NMR (CD_3CN, 400 MHz) of **1b**:



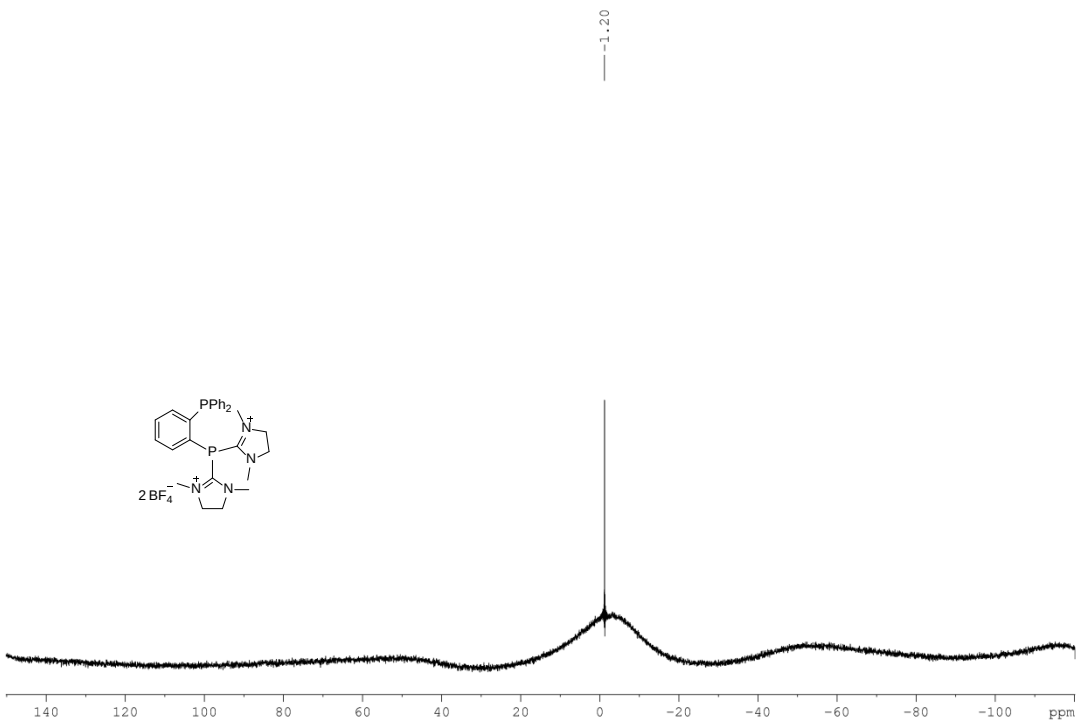
^{13}C NMR (CD_3CN, 100 MHz) of **1b**:



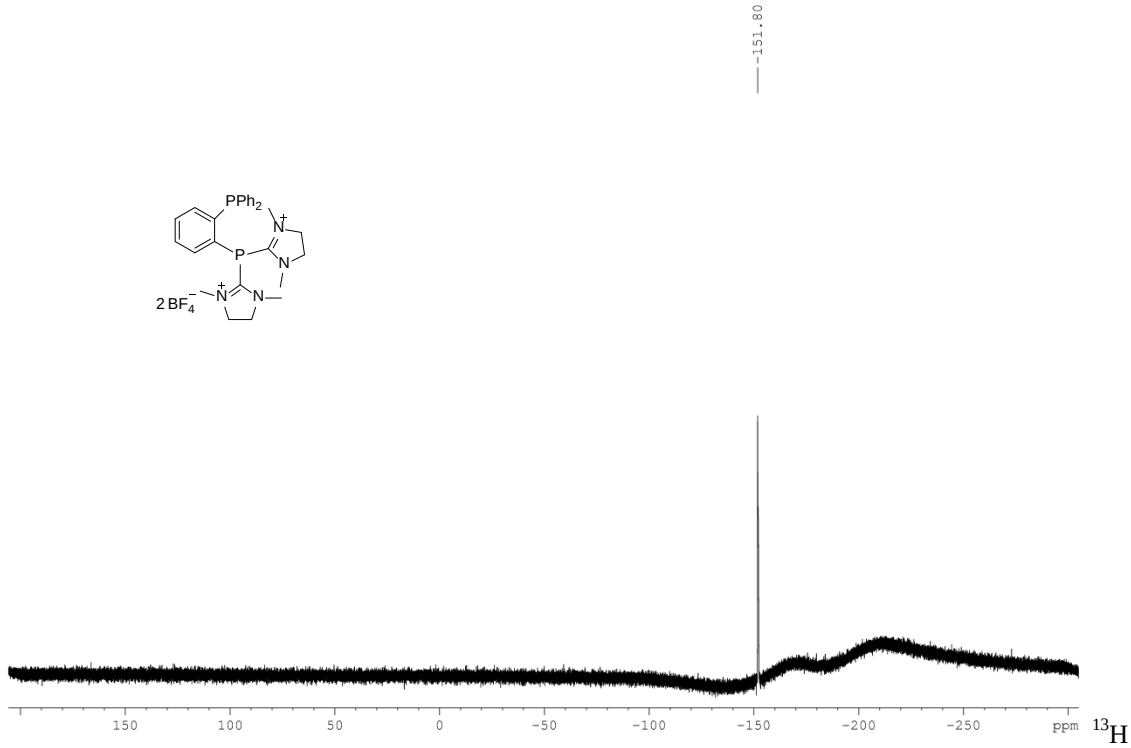
^{31}P NMR ($CDCl_3$, 121 MHz) of **1b**:



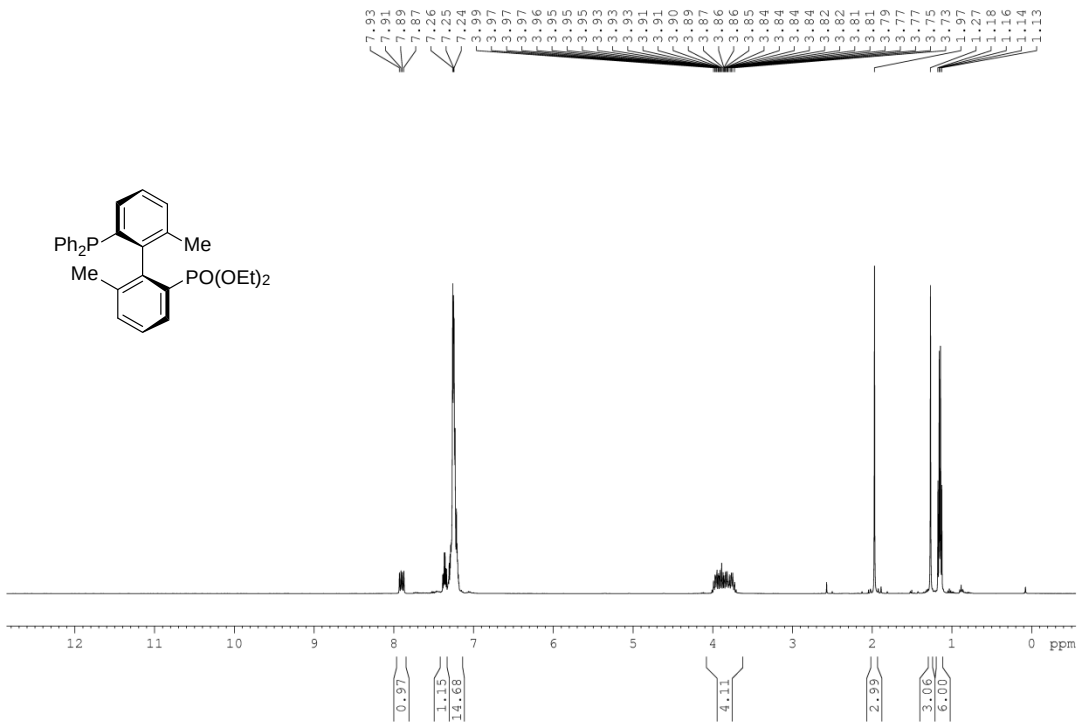
^{11}B NMR (CD_3CN, 96 MHz) of **1b**:



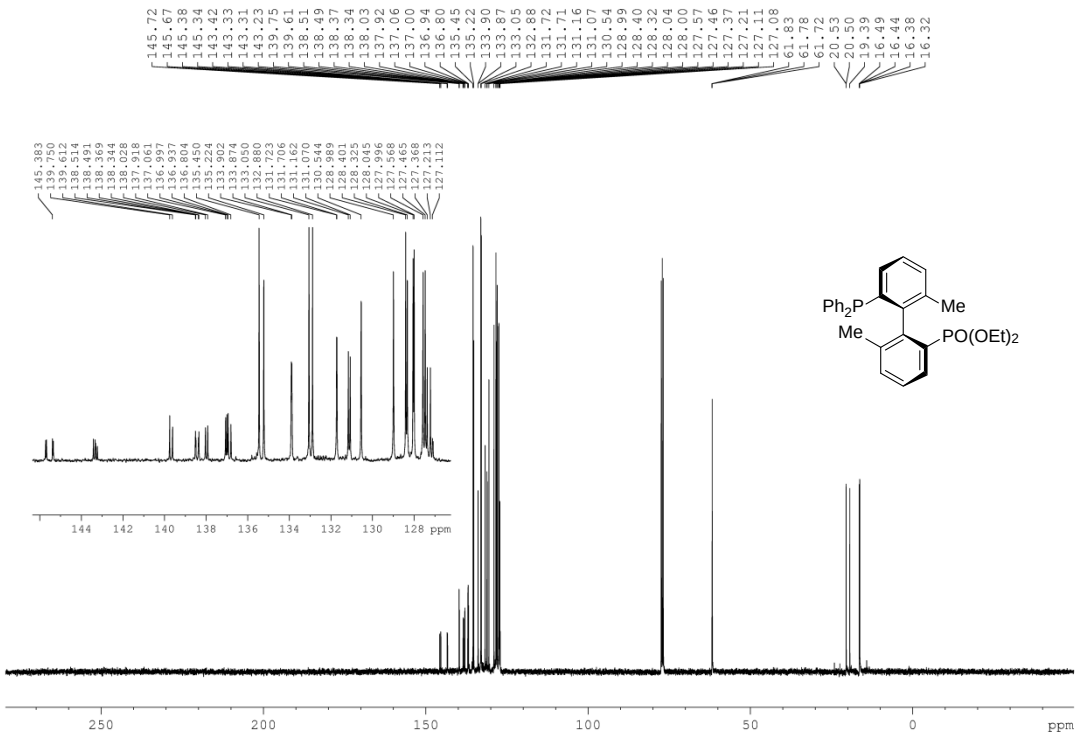
^{19}F NMR (CD_3CN, 282 MHz) of **1b**:



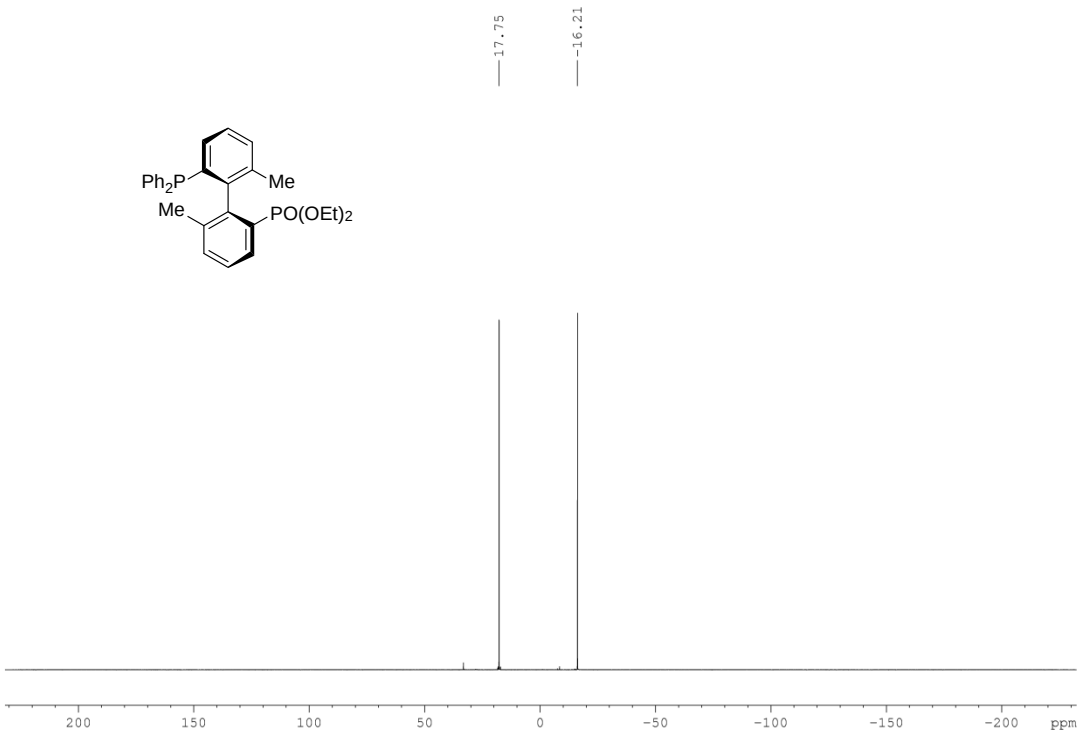
^{1}H NMR ($CDCl_3$, 400 MHz):



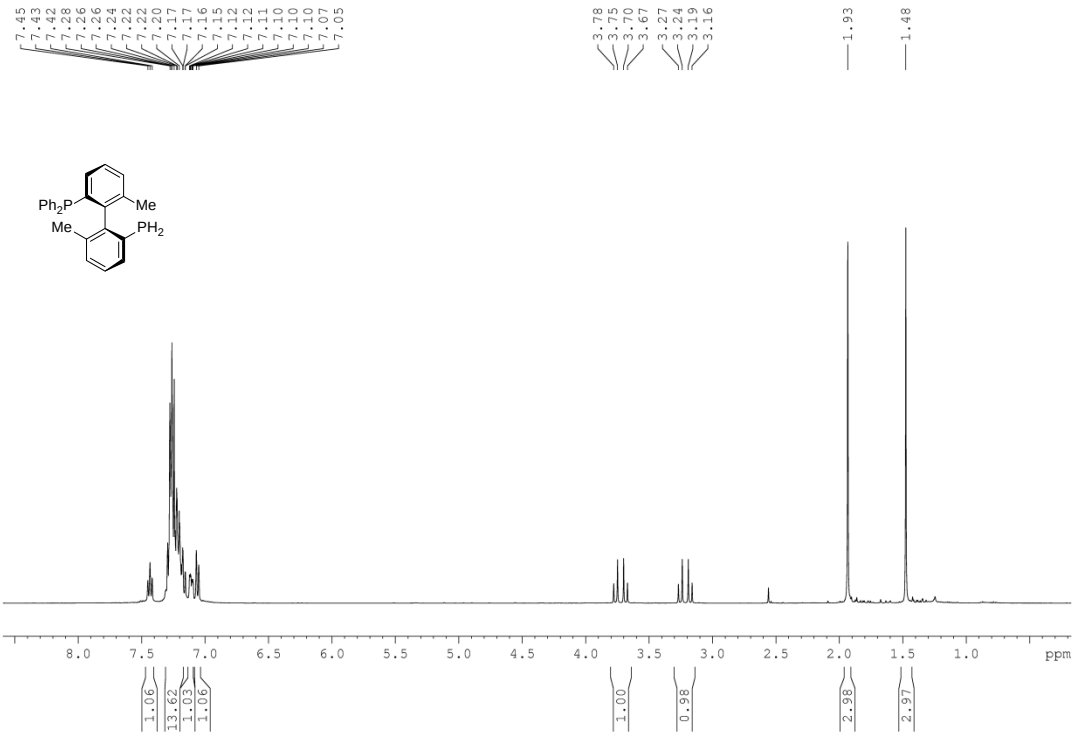
^{13}C NMR ($CDCl_3$, 100 MHz):



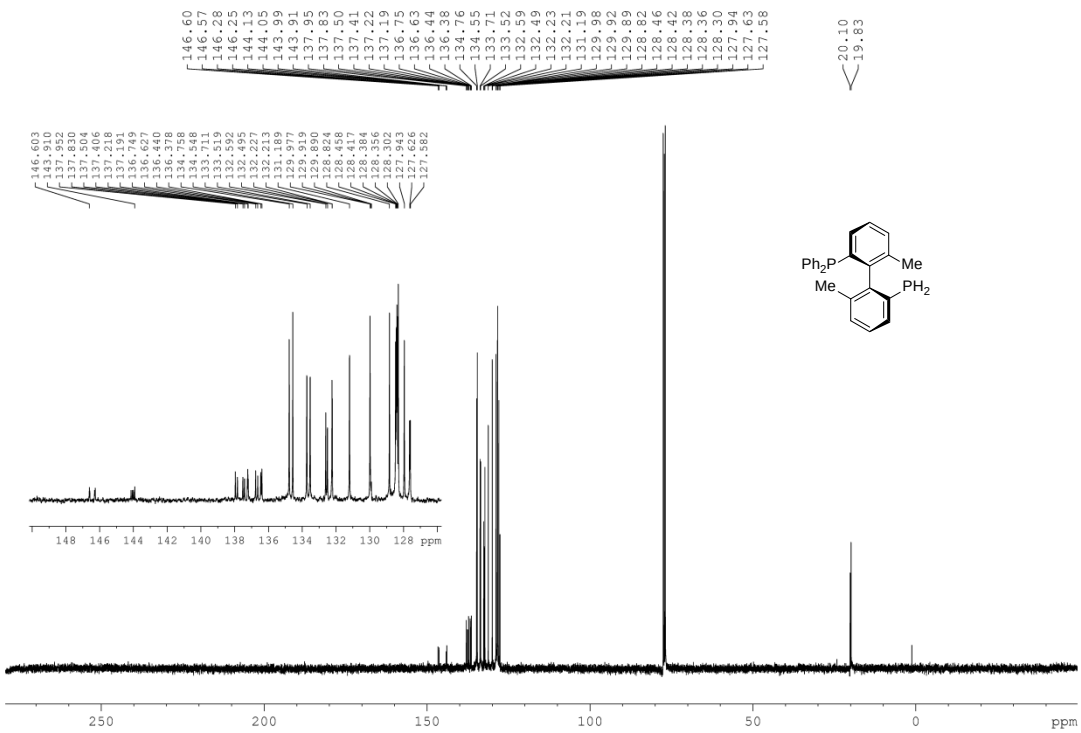
^{31}P NMR ($CDCl_3$, 121 MHz):



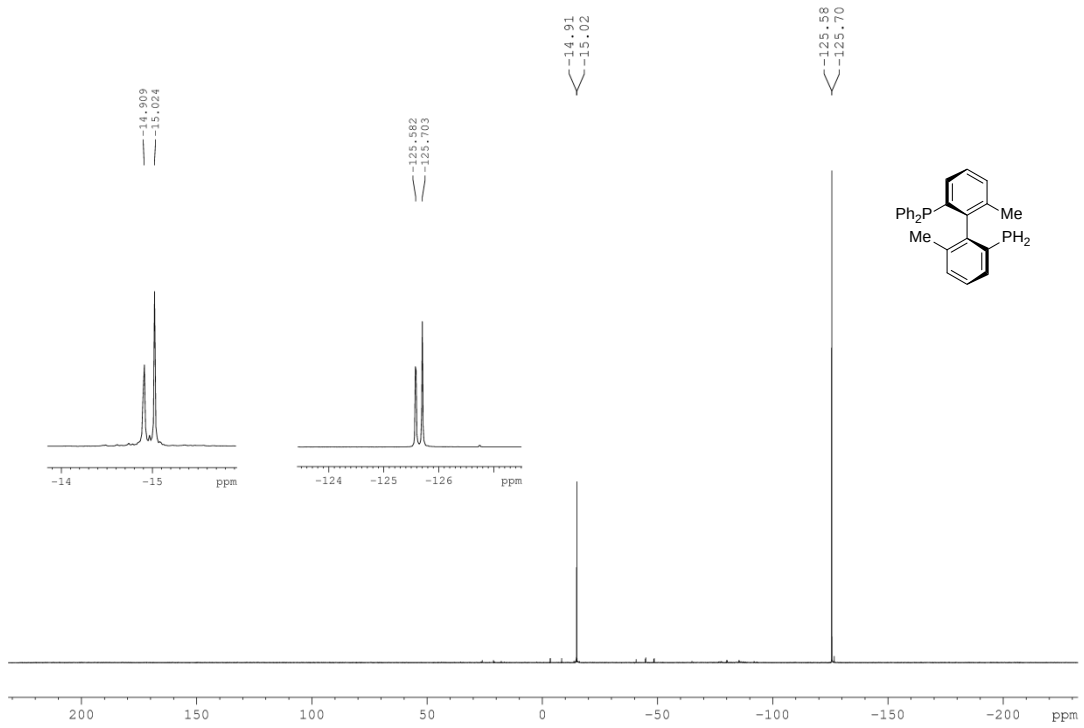
^{1}H NMR ($CDCl_3$, 400 MHz) of **5**:



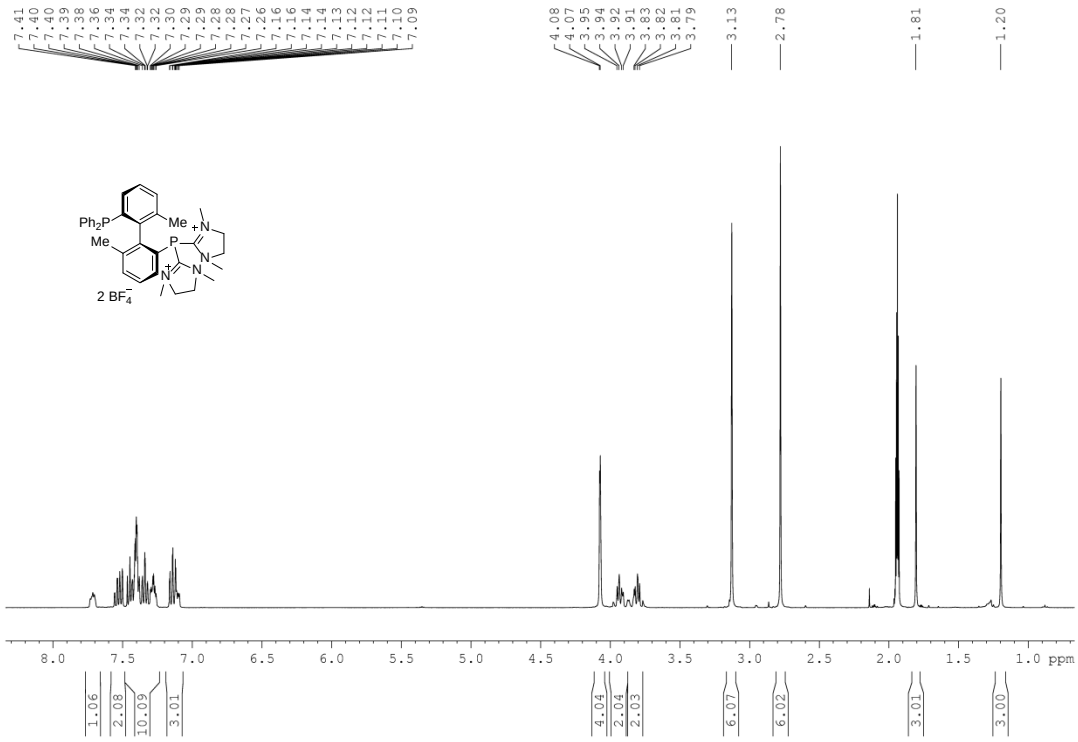
^{13}C NMR ($CDCl_3$, 100 MHz) of **5**:



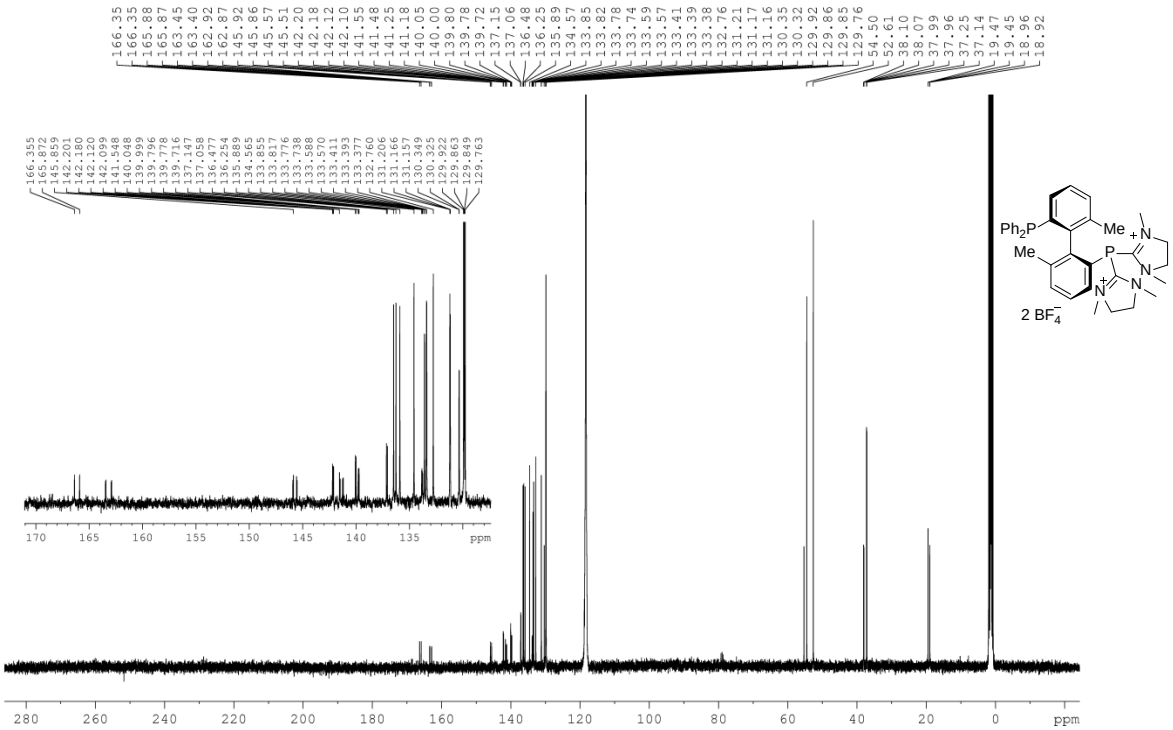
^{31}P NMR ($CDCl_3$, 121 MHz) of **5**:



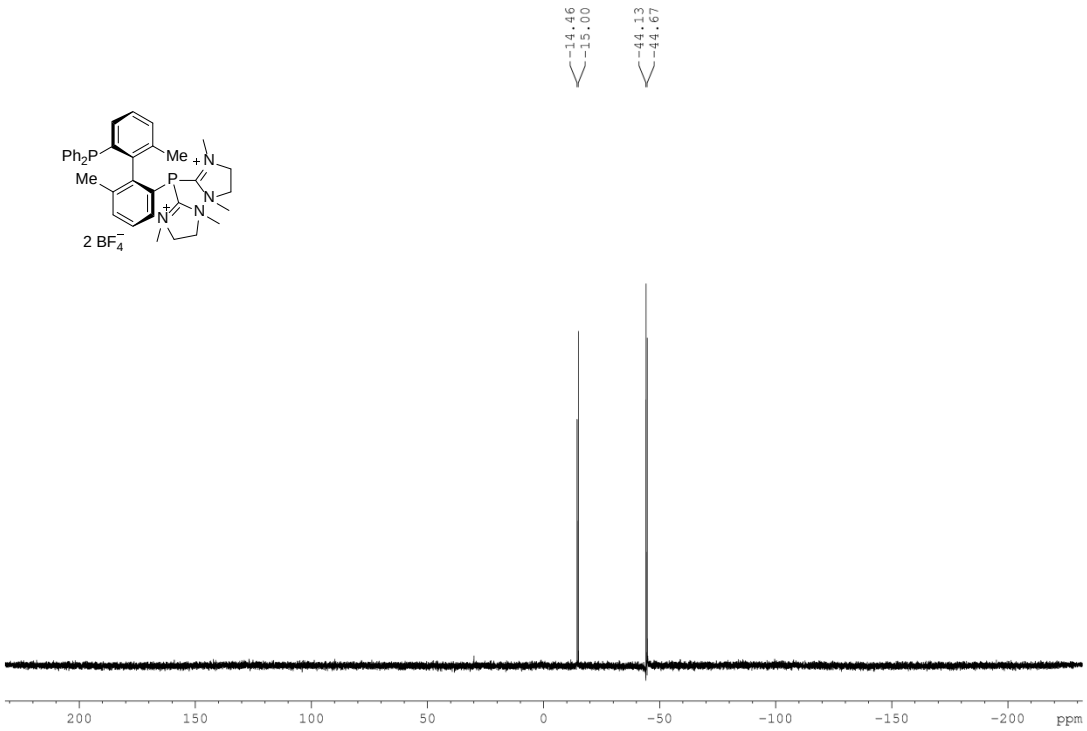
^{1}H NMR (CD_3CN, 400 MHz) of **2**:



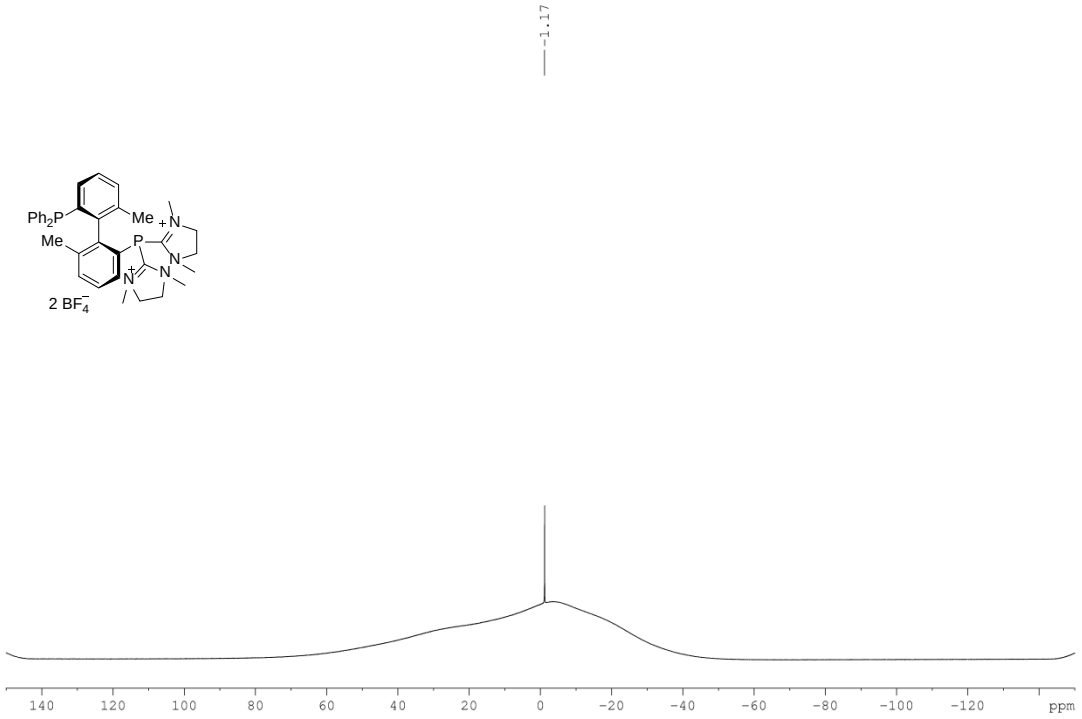
^{13}C NMR (CD_3CN, 100 MHz) of **2**:



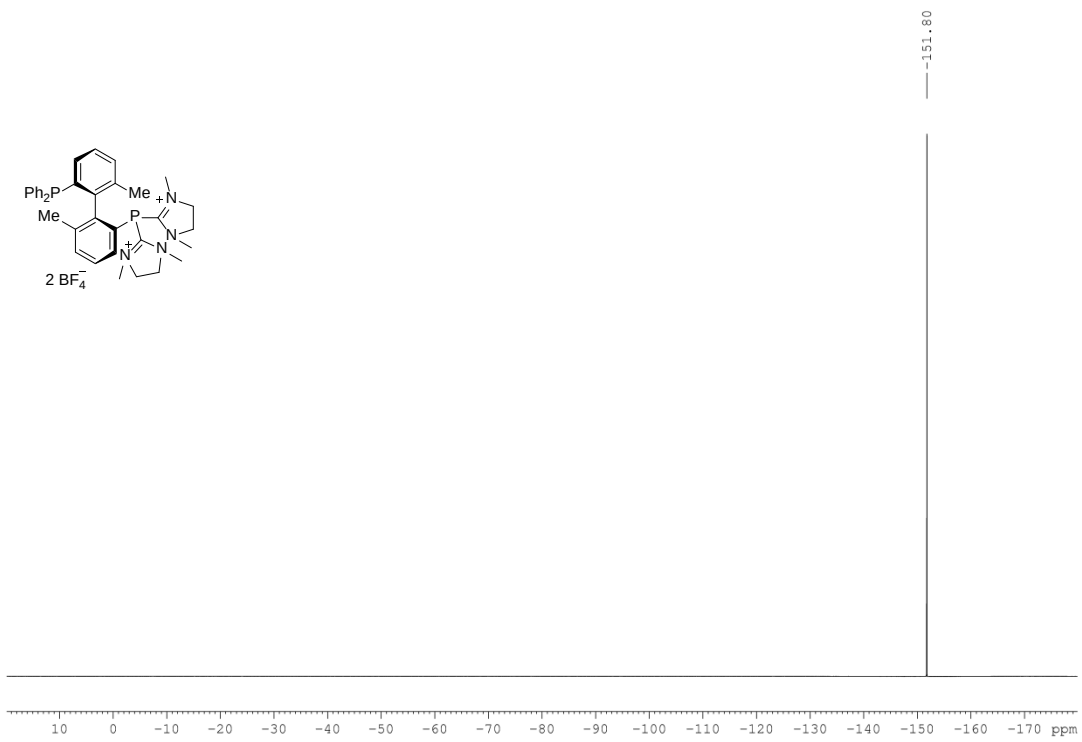
^{31}P NMR (CD_3CN, 121 MHz) of **2**:



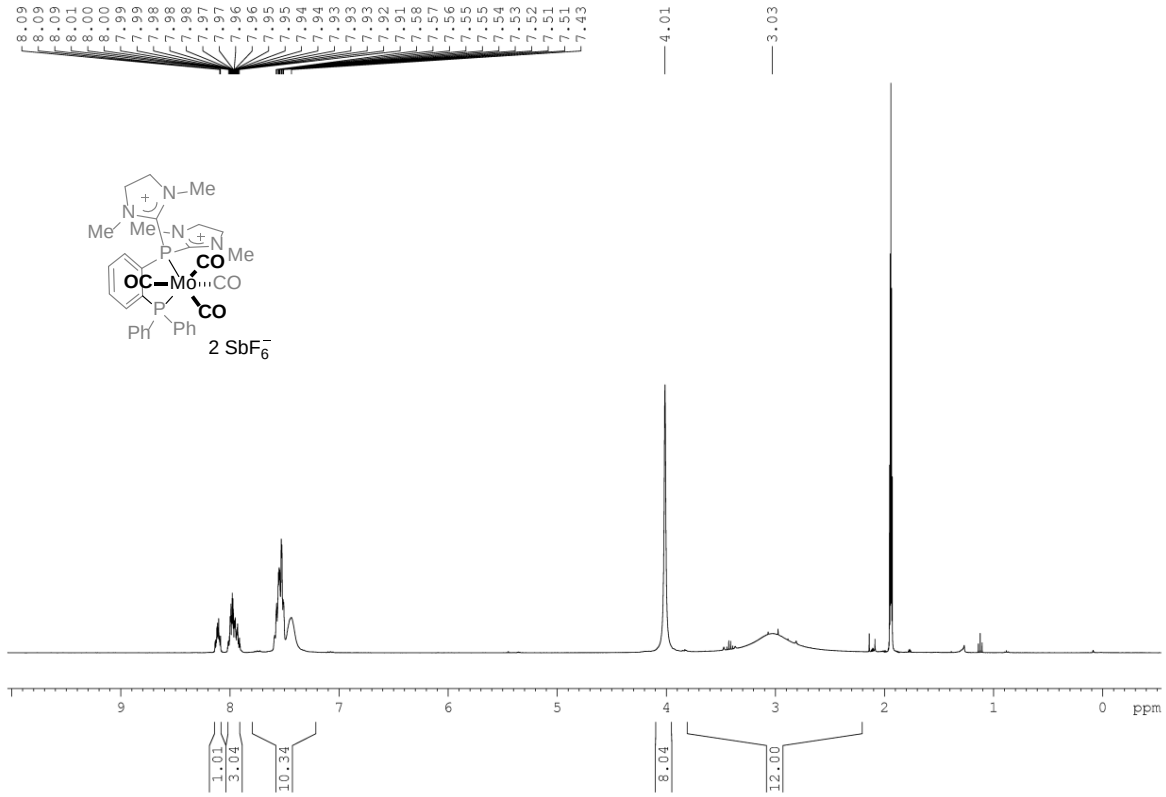
^{11}B NMR (CD_3CN, 96 MHz) of **2**:



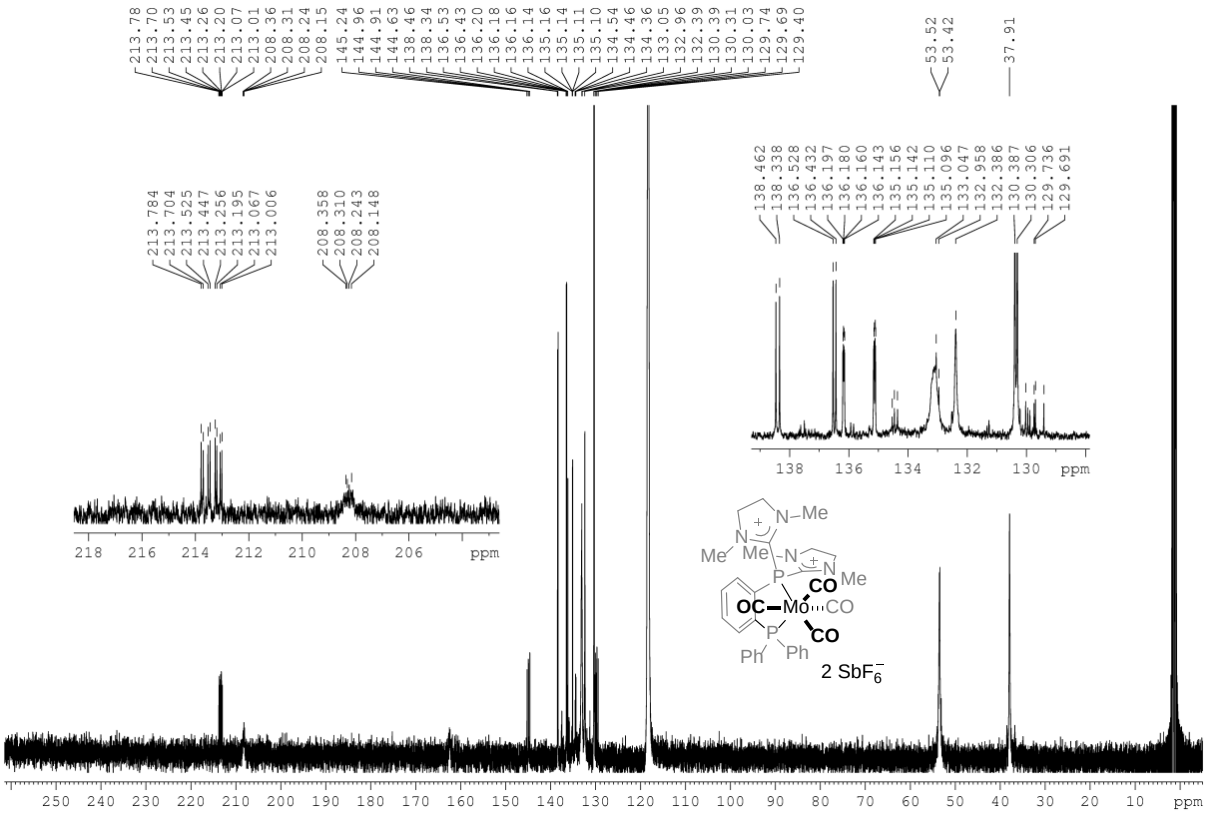
^{19}F NMR (CD_3CN, 282 MHz) of **2**:



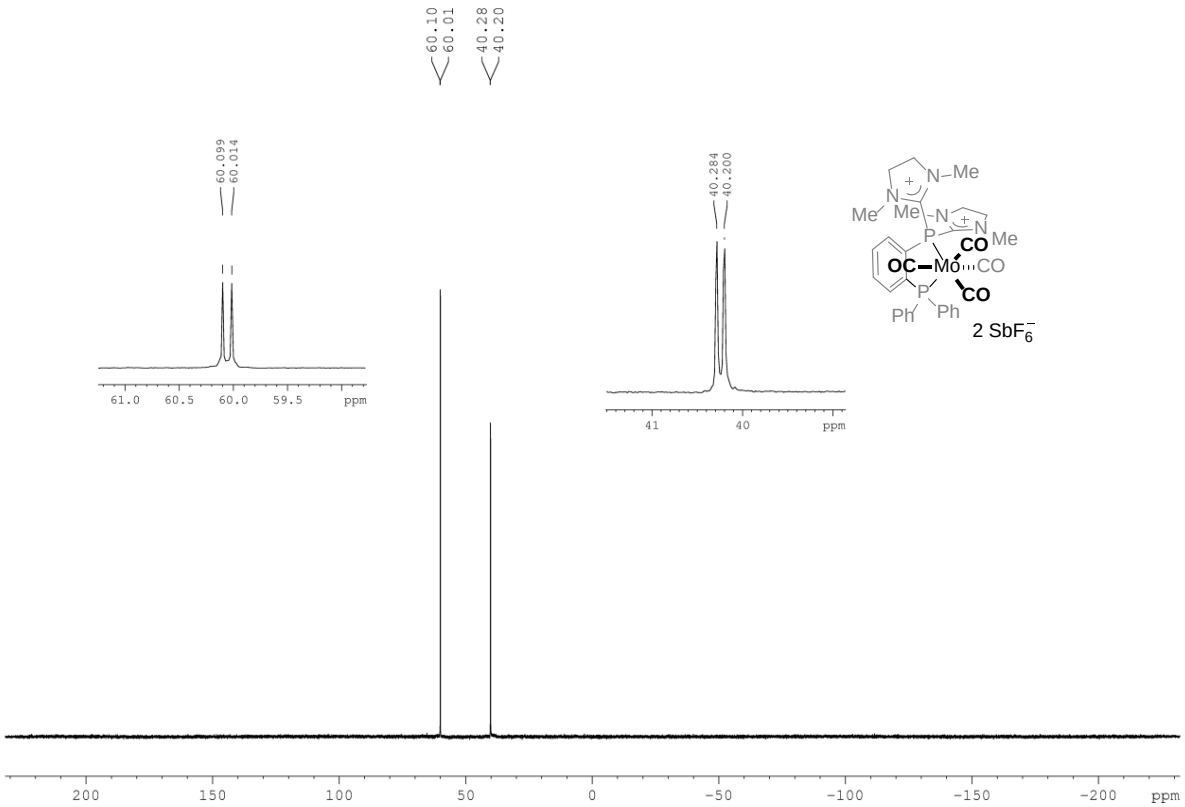
^{1}H NMR (CD_3CN, 400 MHz) of **8:**



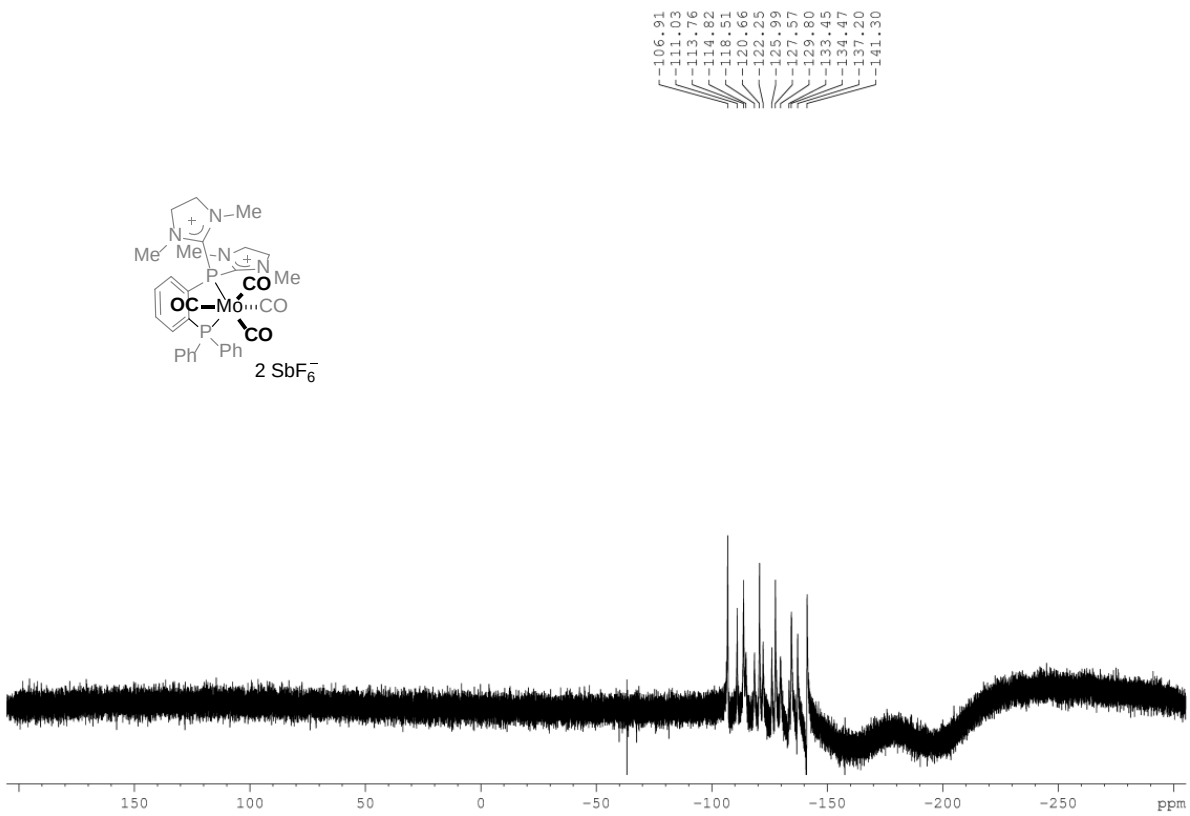
^{13}C NMR (CD_3CN, 125 Mz) of **8**:



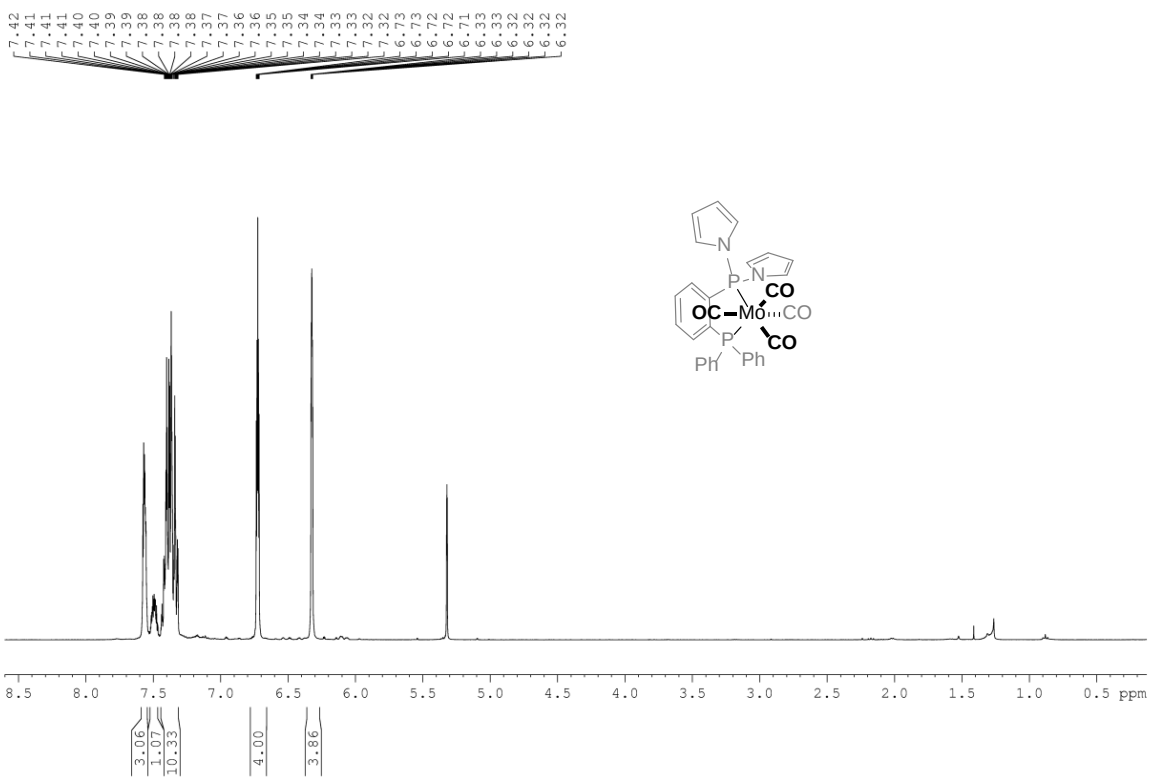
^{31}P NMR (CD_3CN, 162 MHz) of **8**:



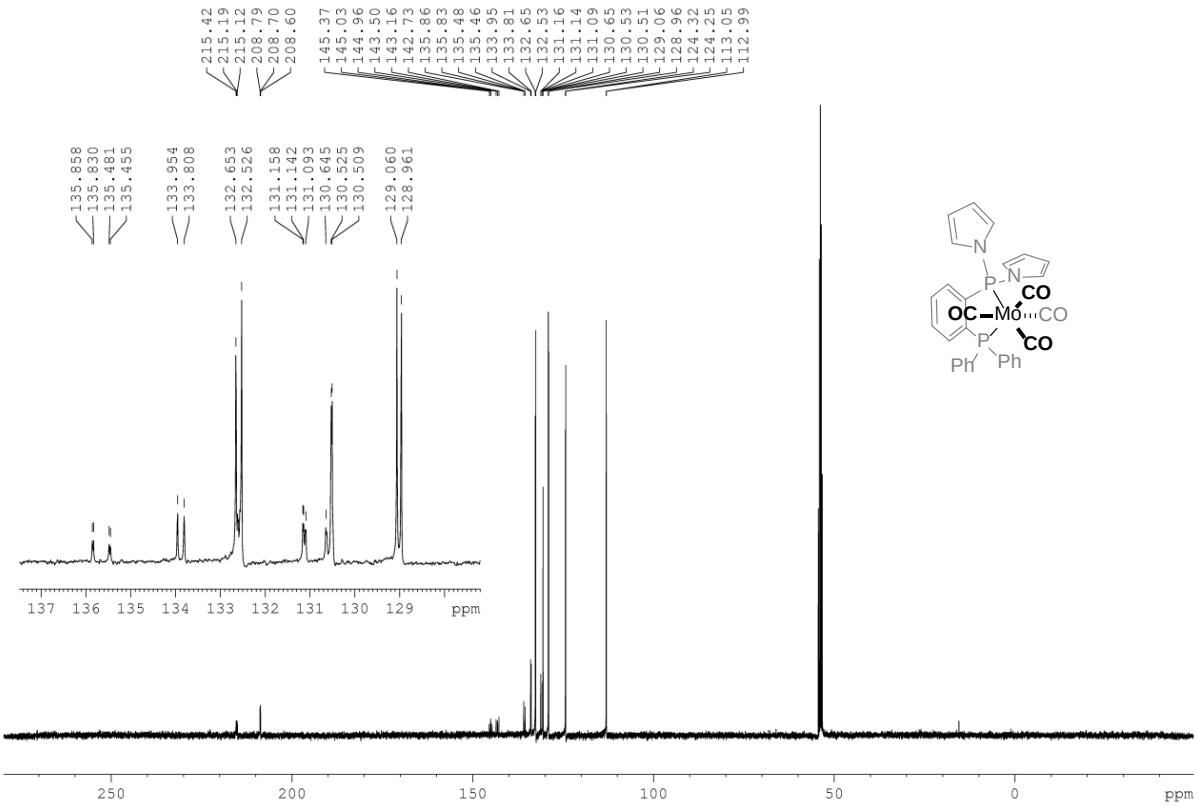
^{19}F NMR (CD_3CN, 282 MHz) of **8**:



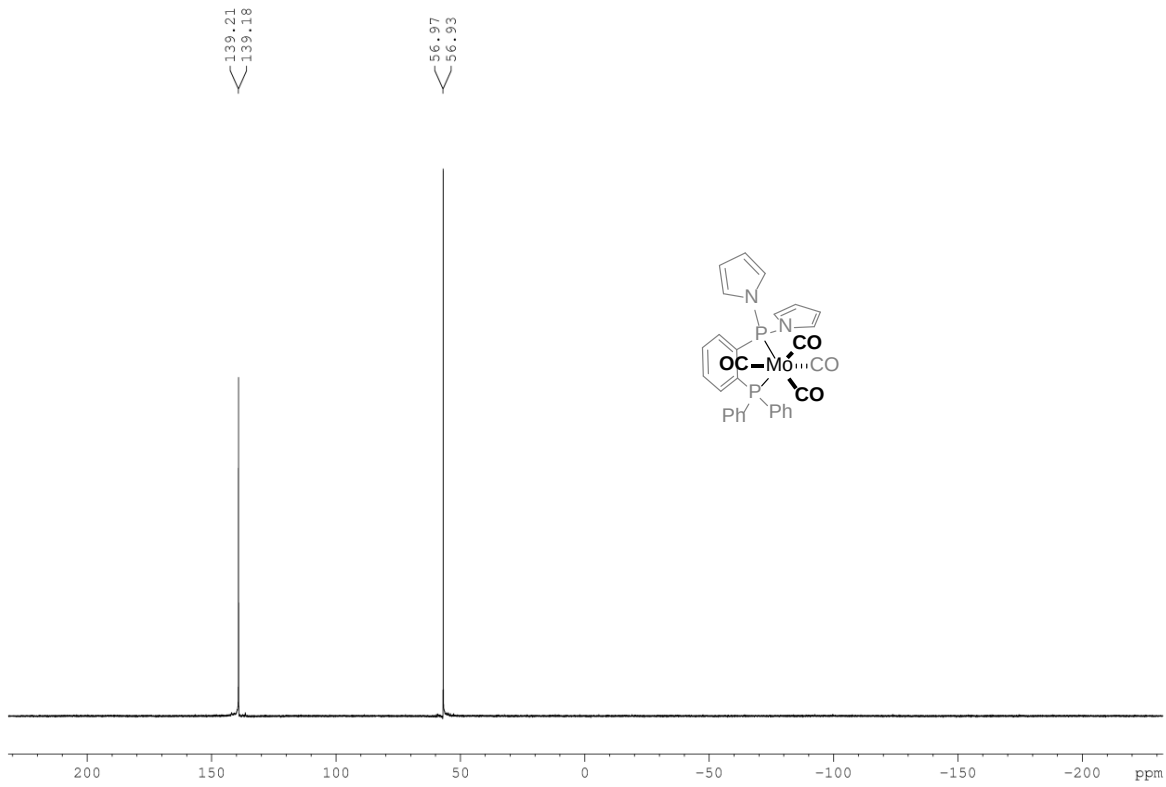
^{1}H NMR (CD_2Cl_2, 400 MHz) of **9**:



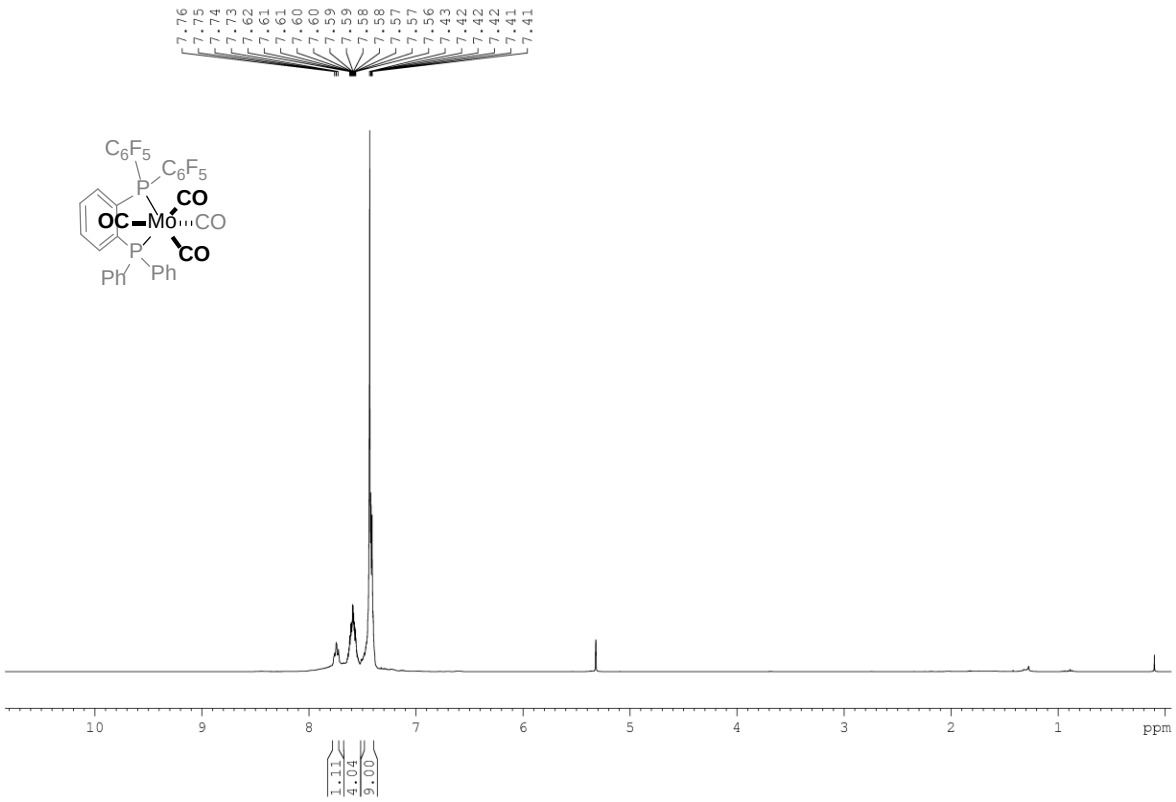
^{13}C NMR (CD_2Cl_2, 100 Mz) of **9**:



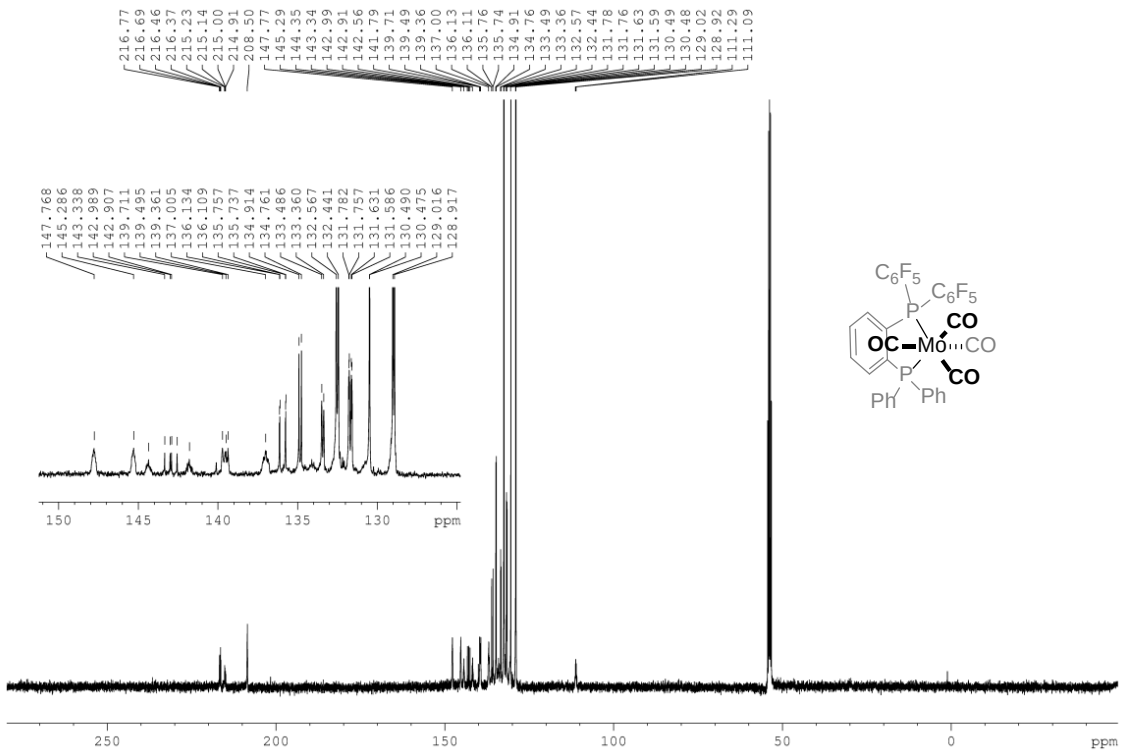
^{31}P NMR (CD_2Cl_2, 162 MHz) of **9**:



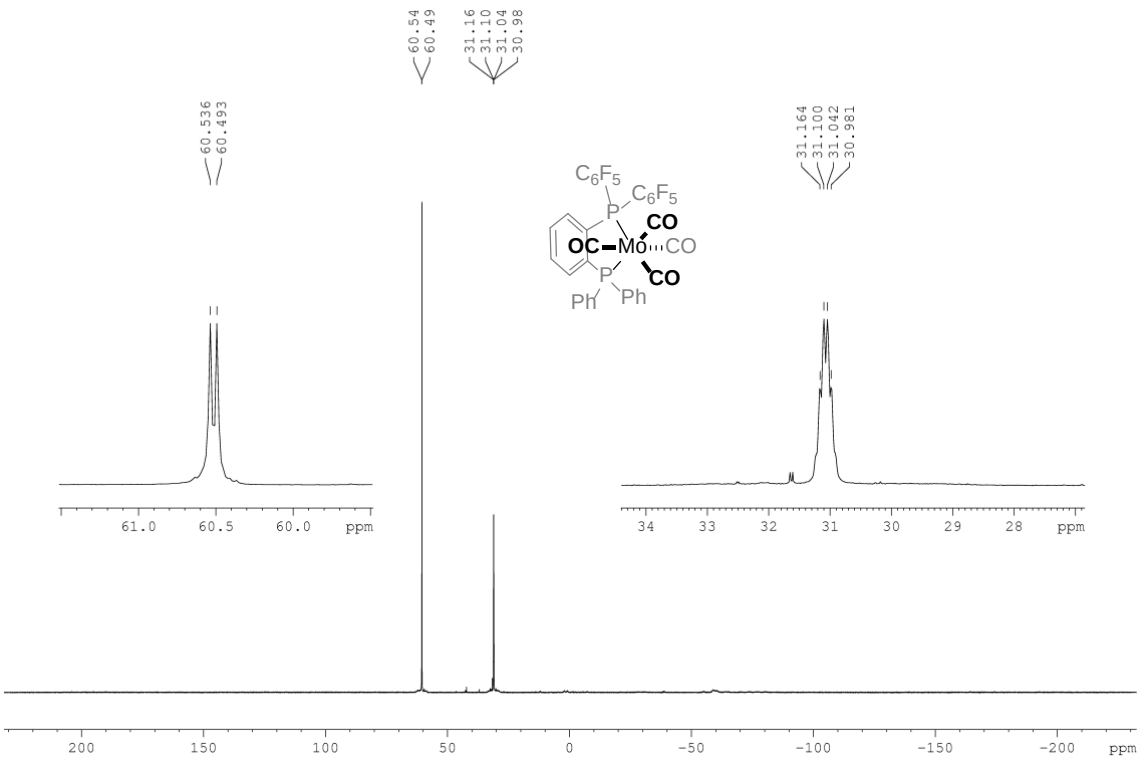
^{1}H NMR (CD_2Cl_2, 400 MHz) of **10**:



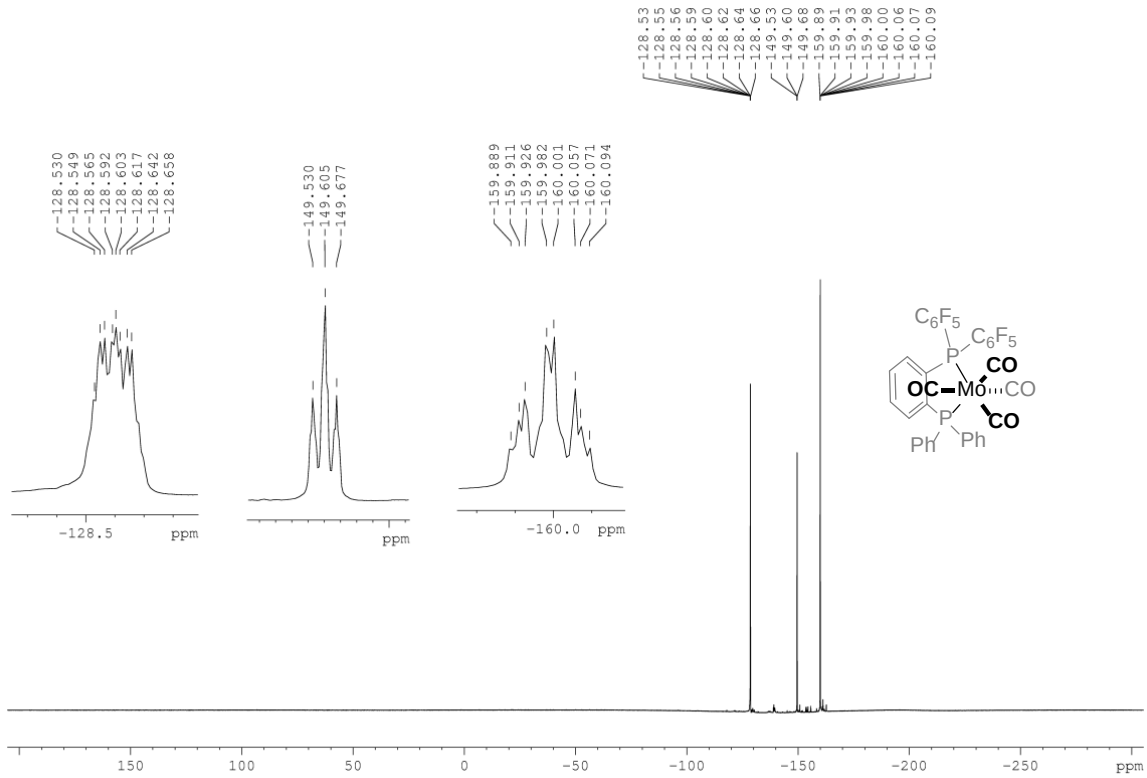
^{13}C NMR (CD_2Cl_2, 100 Mz) of **10**:



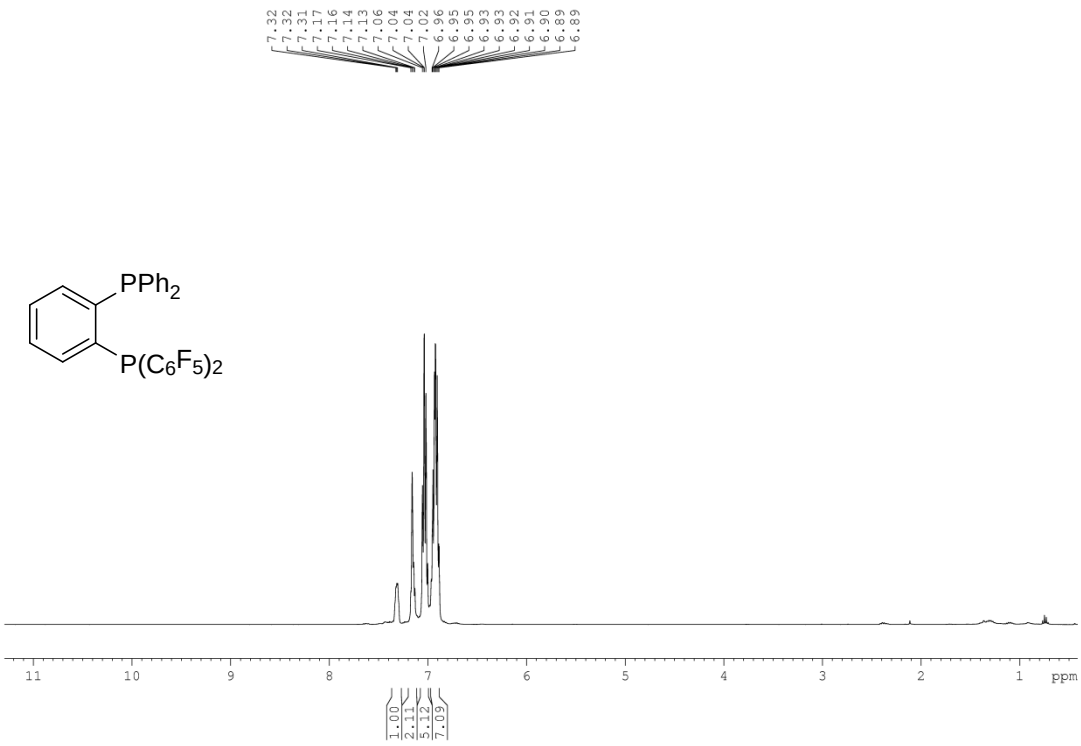
^{31}P NMR (CD_2Cl_2, 162 MHz) of **10**:



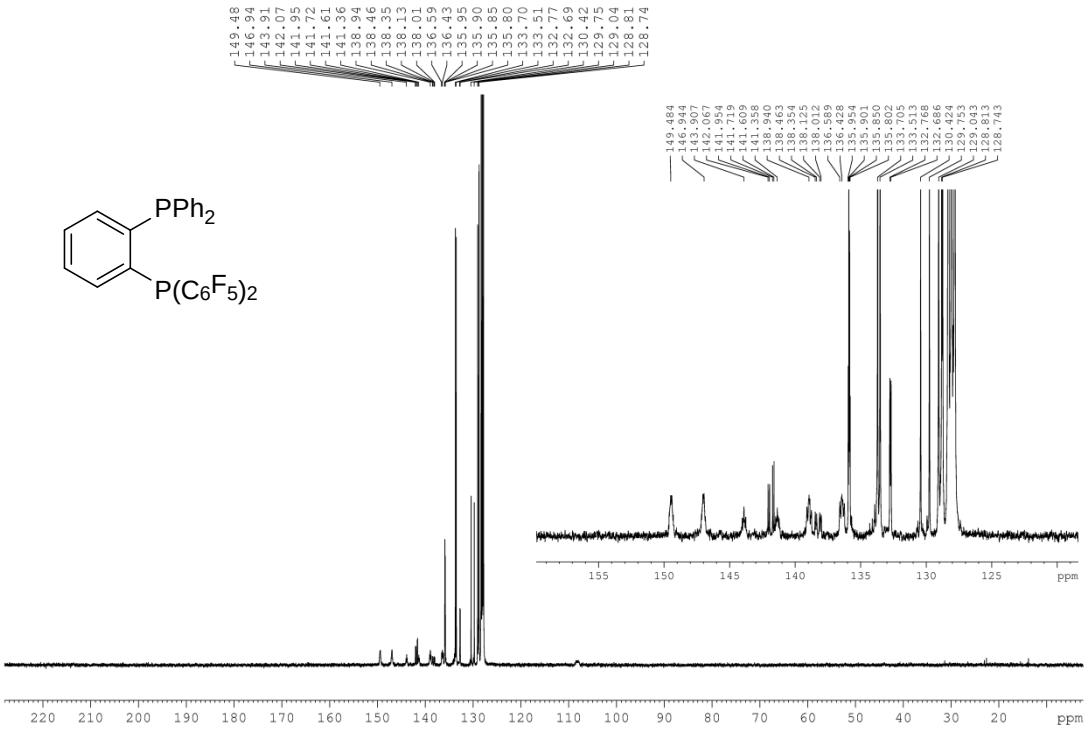
^{19}F NMR (CD_2Cl_2, 282 MHz) of **10**:



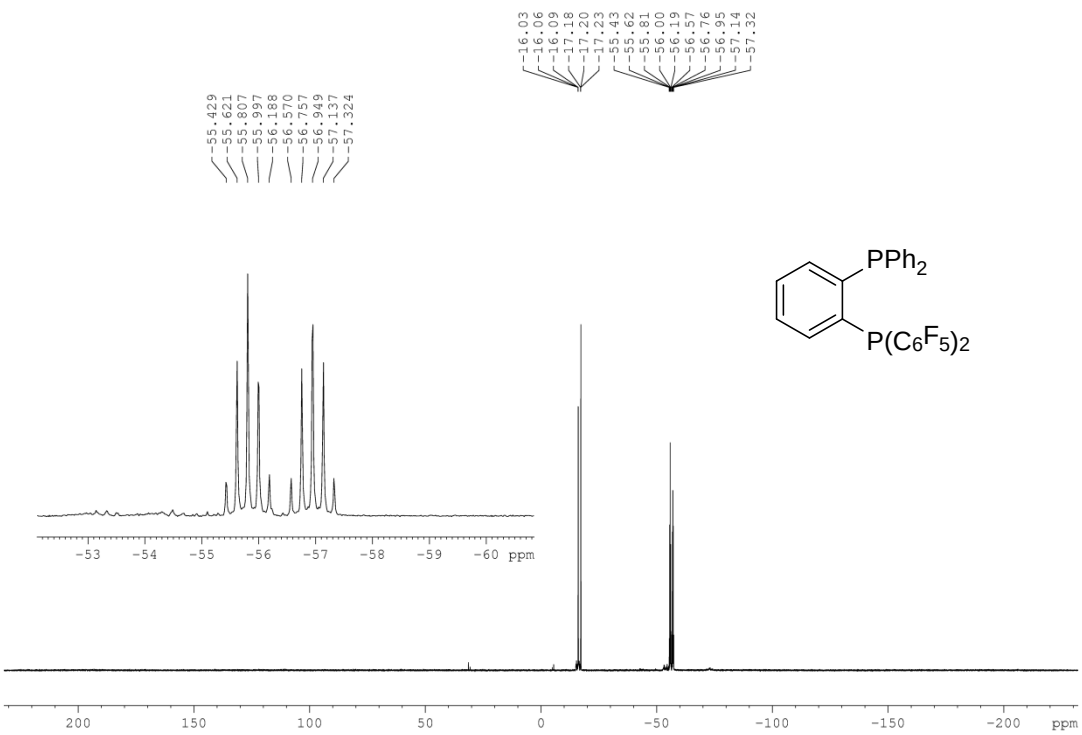
^{1}H NMR (C_6D_6, 400 MHz) of **12**:



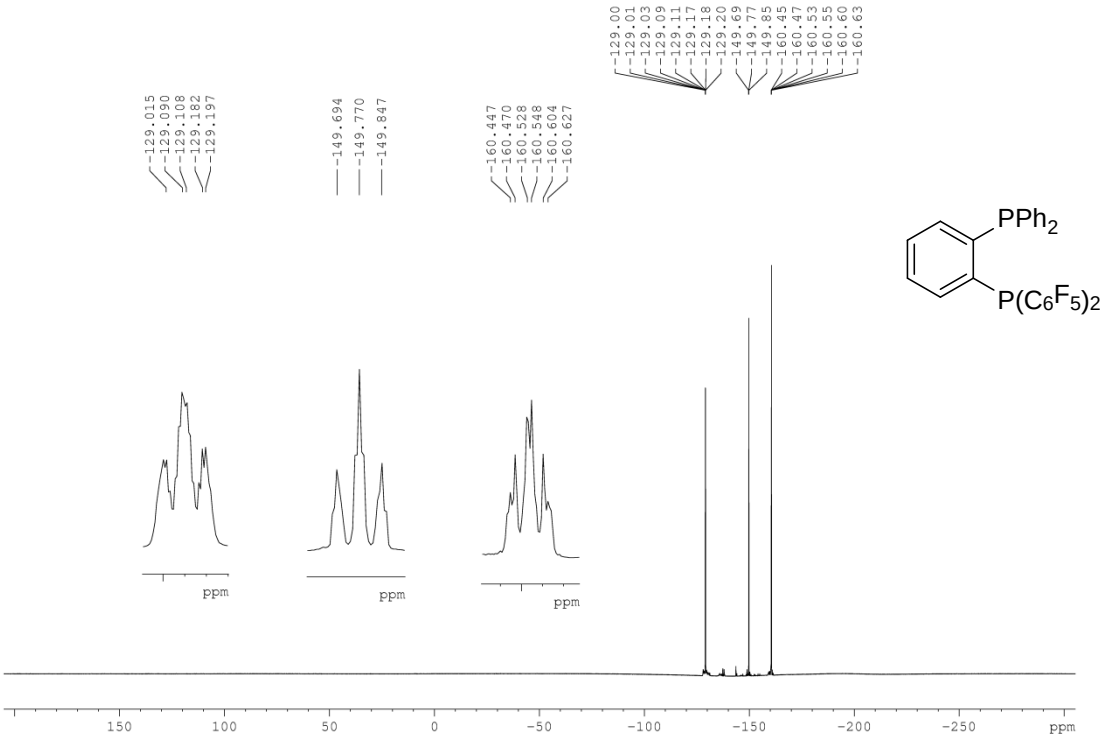
^{13}C NMR (C_6D_6, 100 MHz) of **12**:



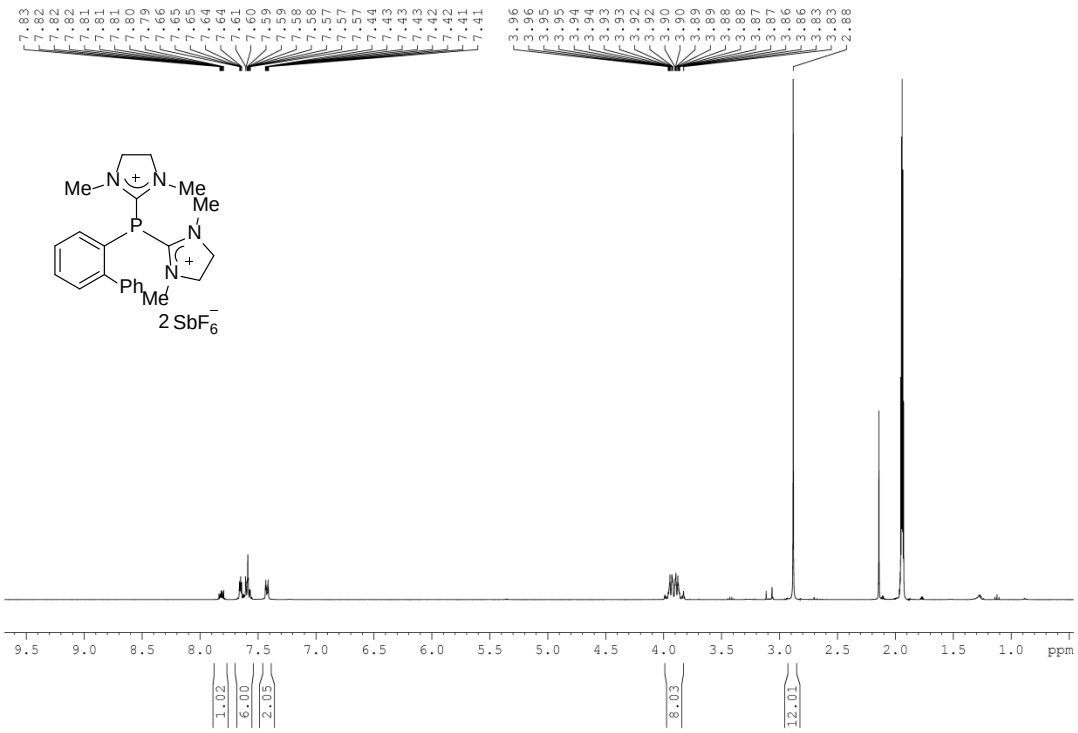
^{31}P NMR (C_6D_6, 121 MHz) of **12**:



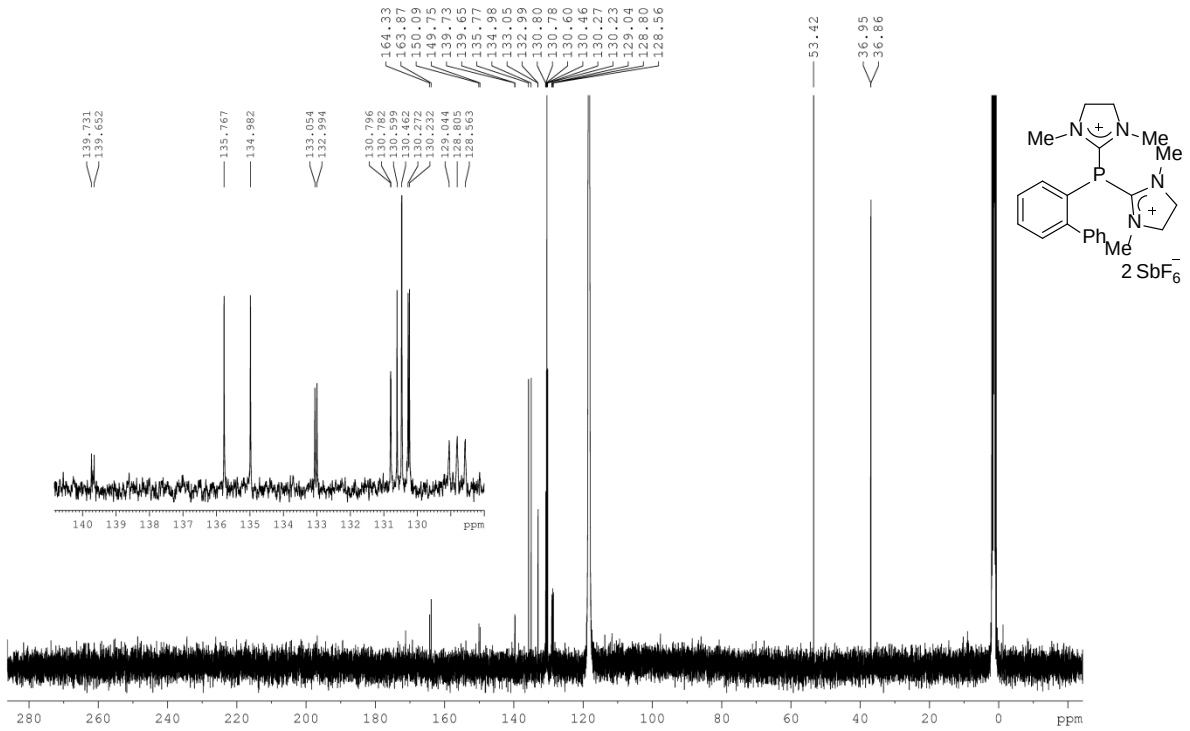
^{19}F NMR (C_6D_6, 282 MHz) of **12**:



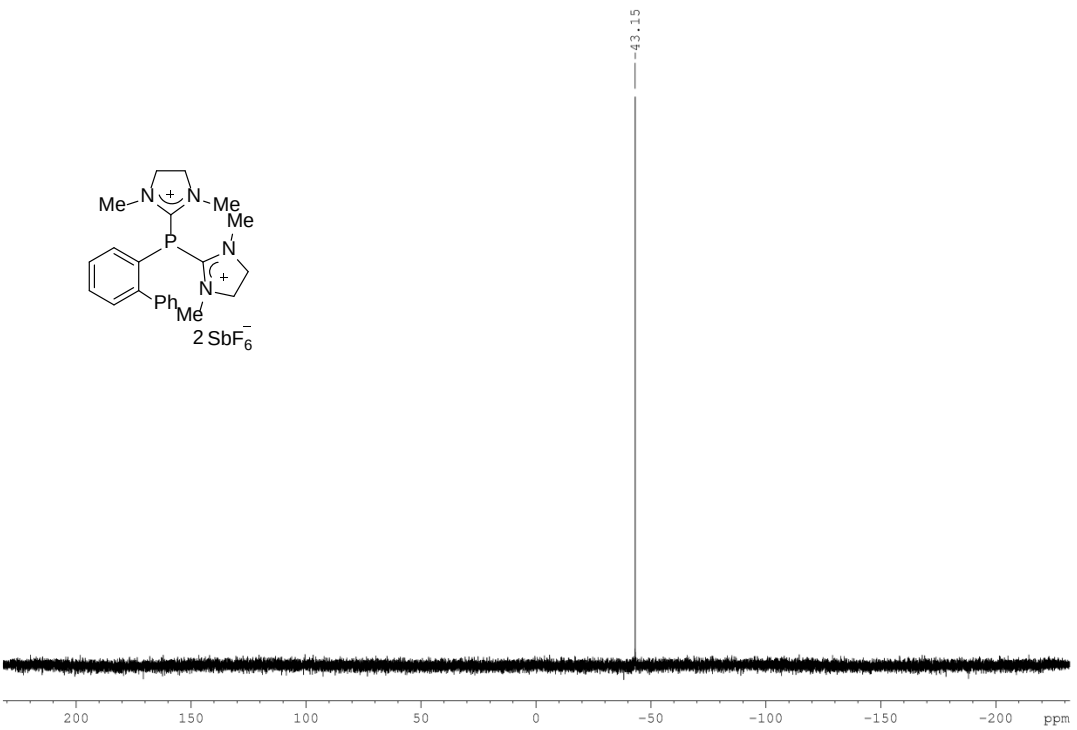
^{1}H NMR (CD_3CN, 400 MHz) of **13**:



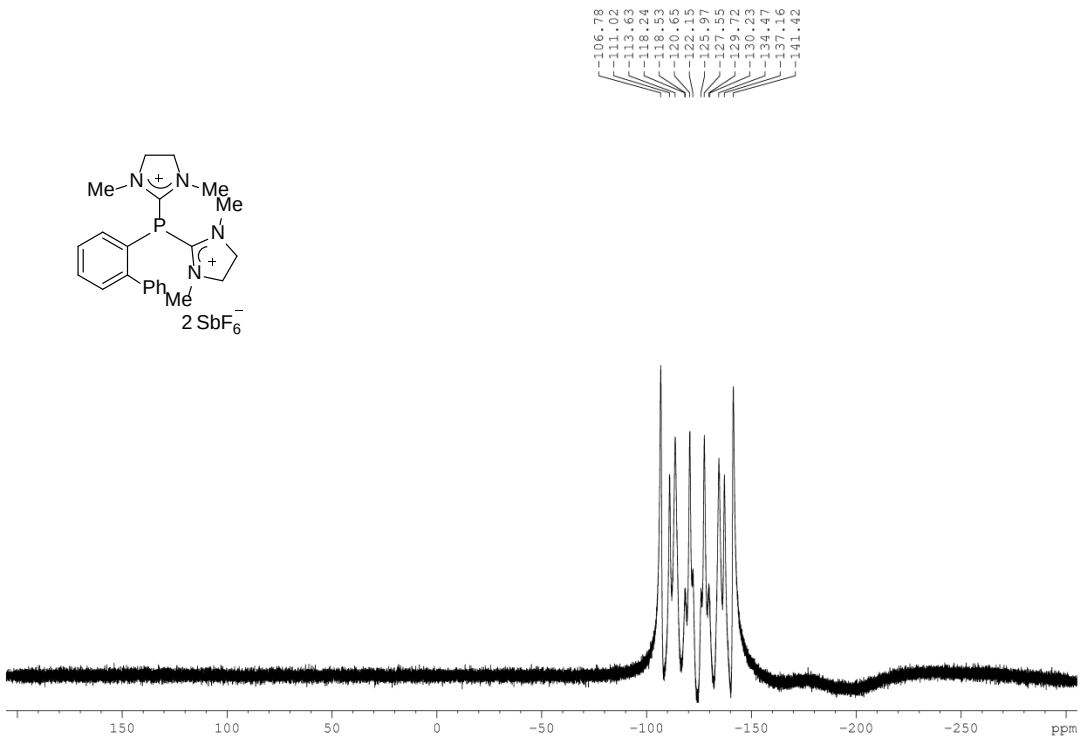
^{13}C NMR (CD_3CN, 100 MHz) of **13**:



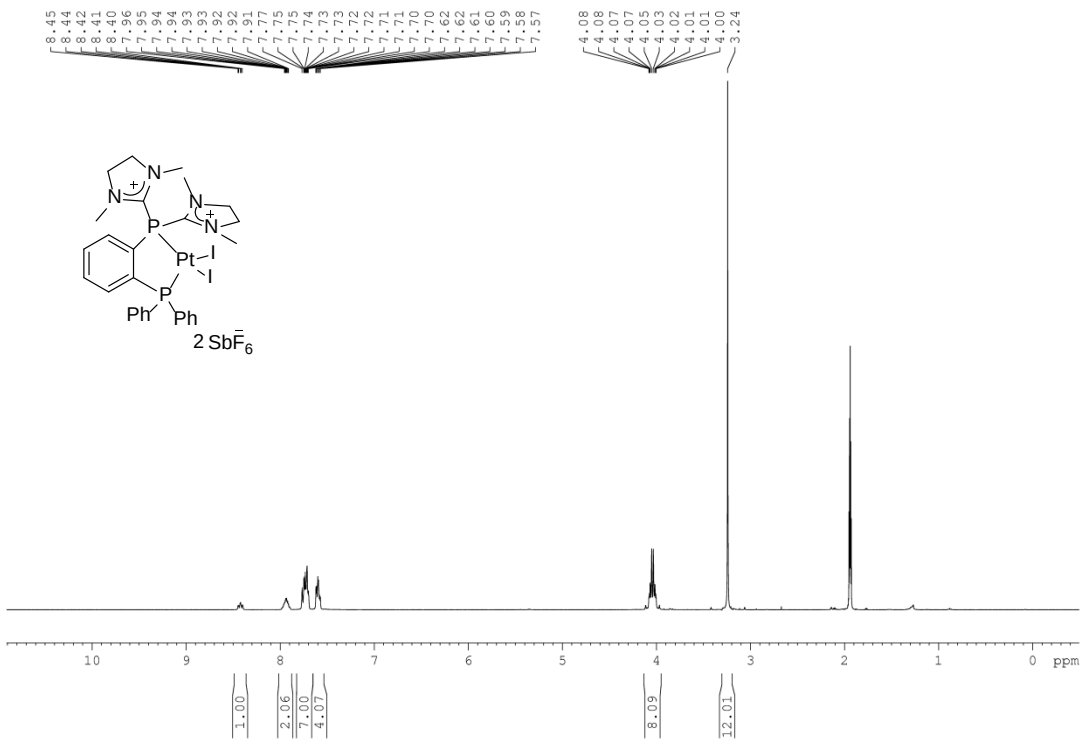
^{31}P NMR (CD_3CN, 121 MHz) of **13**:



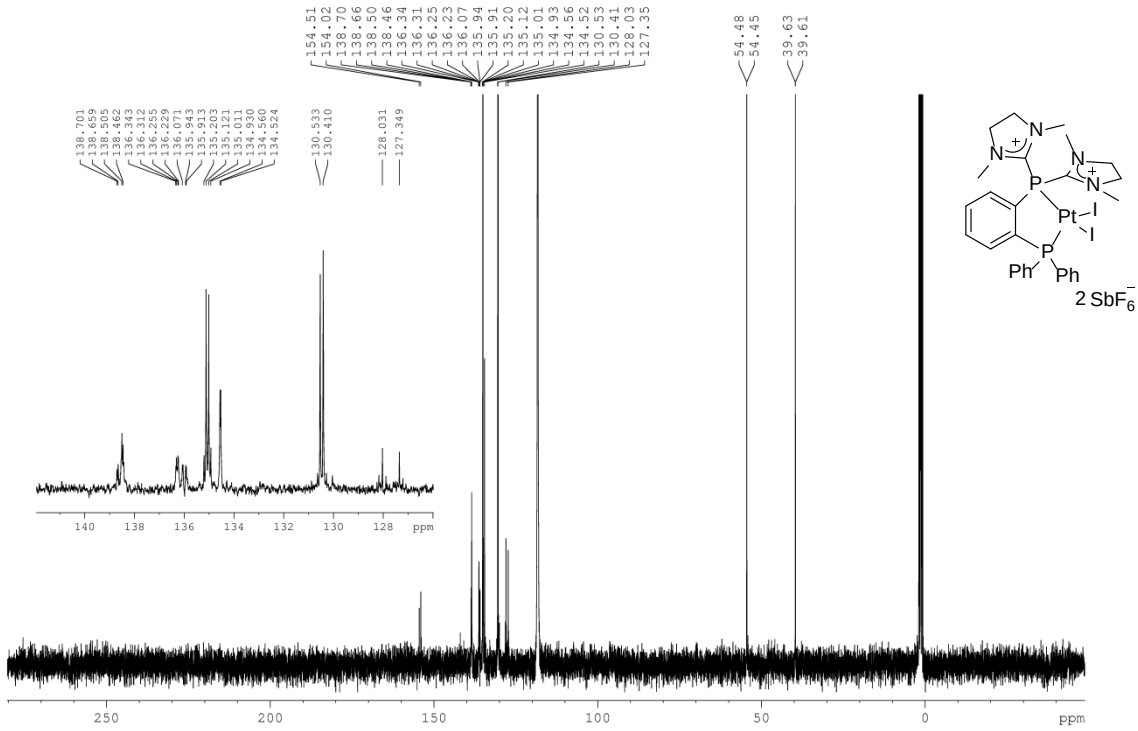
^{19}F NMR (CD_3CN, 282 MHz) of **13**:



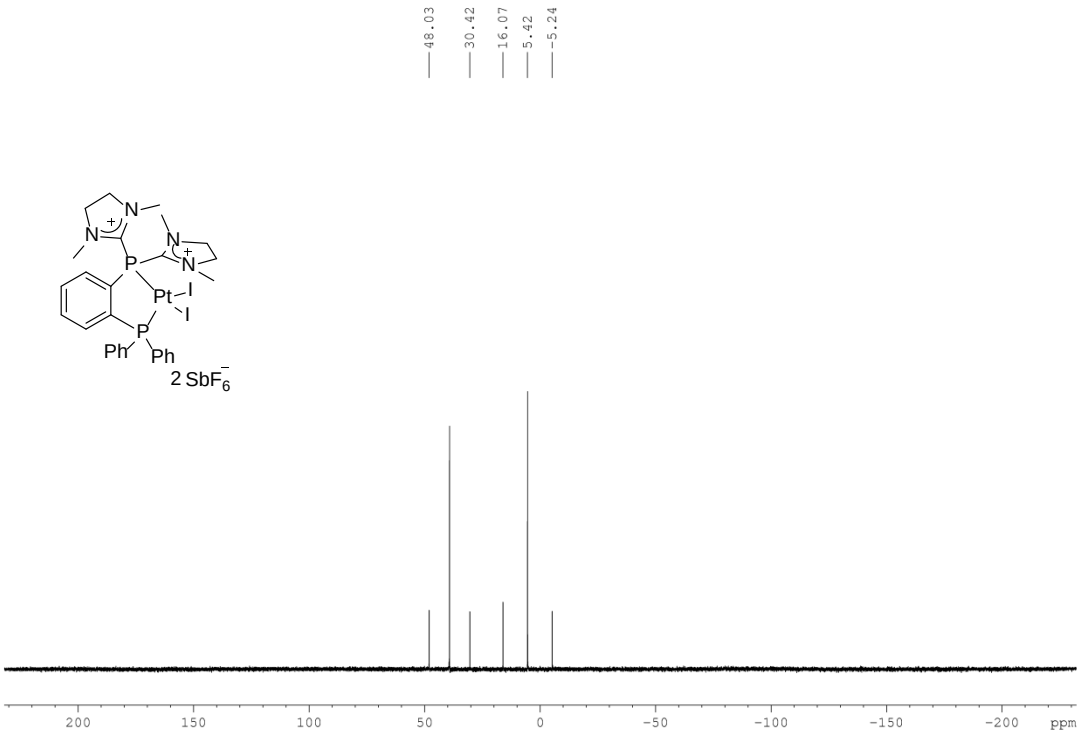
^{1}H NMR (CD_3CN, 400 MHz) of **17**:



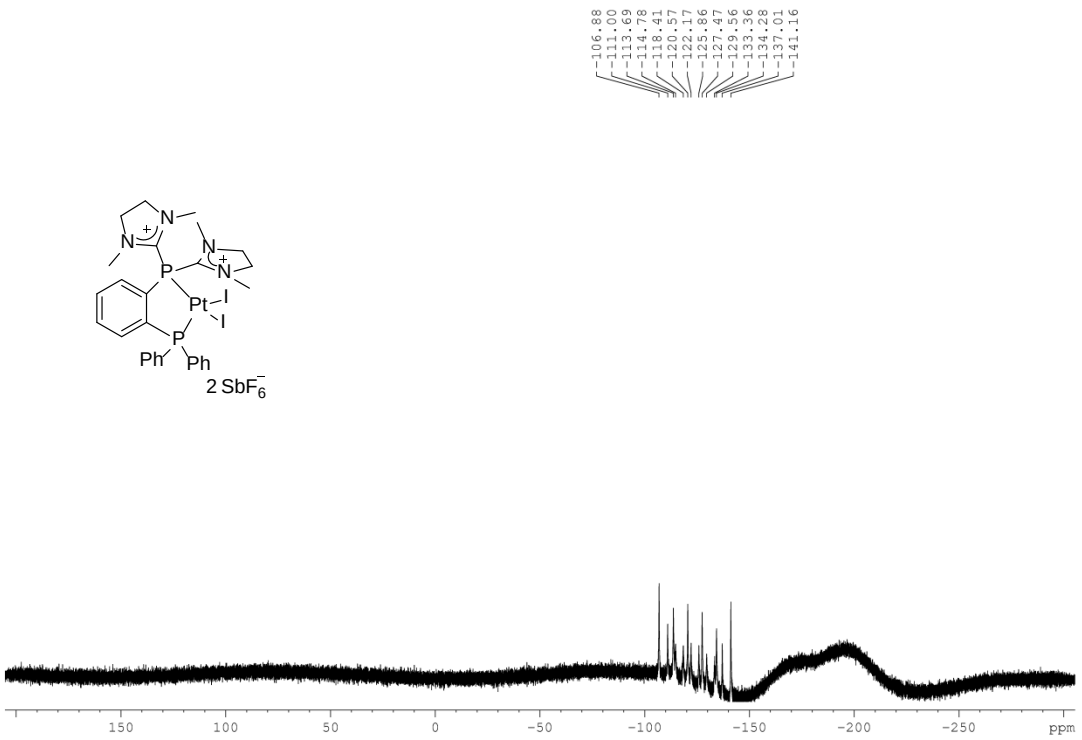
^{13}C NMR (CD_3CN, 100 MHz) of **17**:



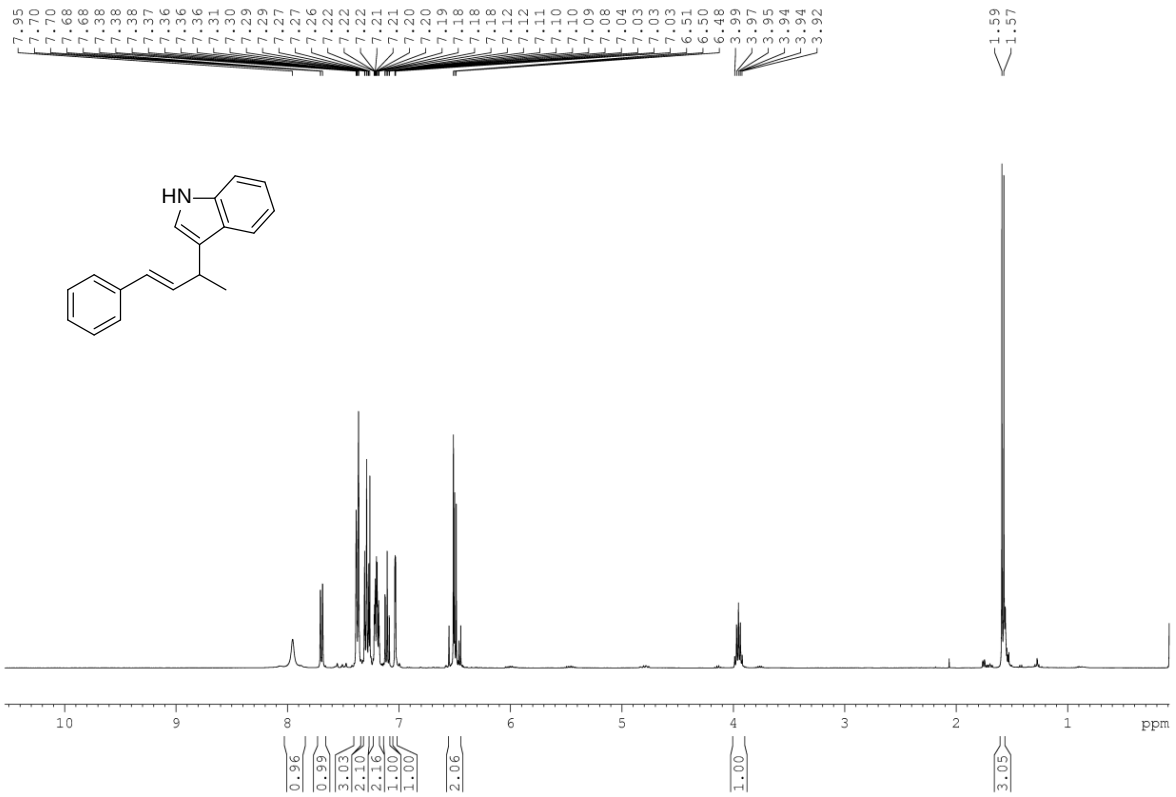
^{31}P NMR (CD_3CN, 121 MHz) of **17**:



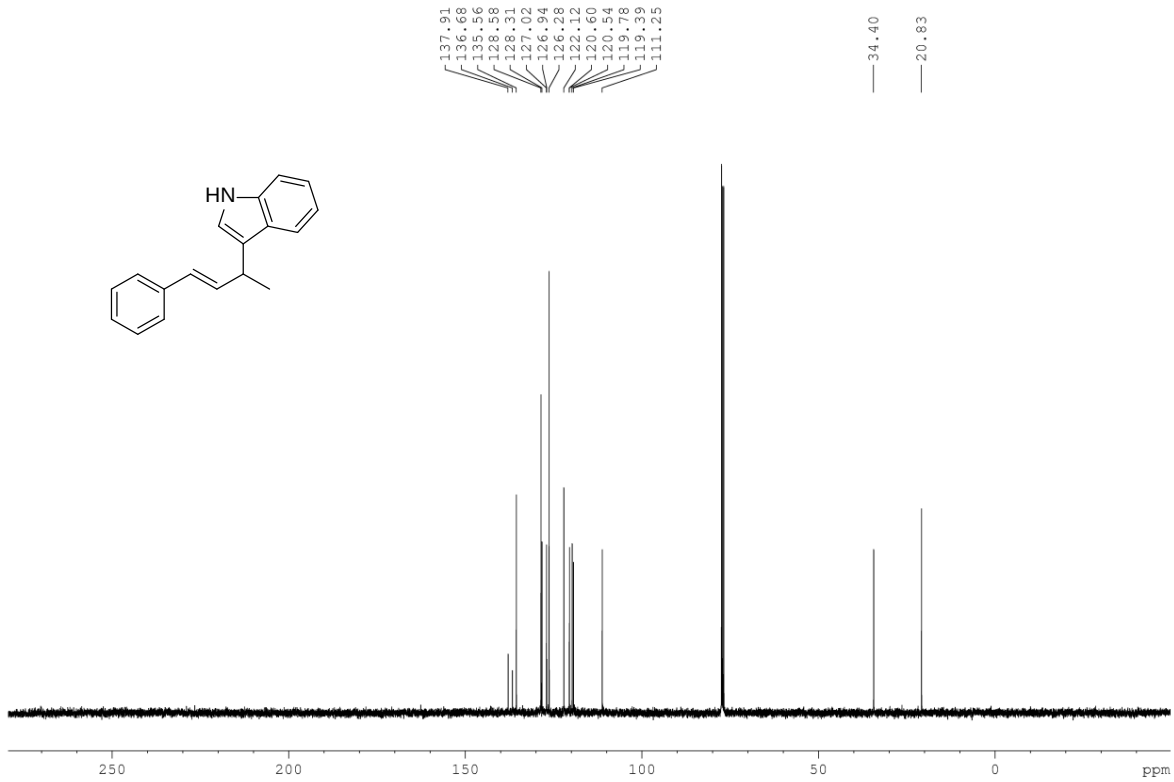
^{19}F NMR (CD_3CN, 282 MHz) of **17**:



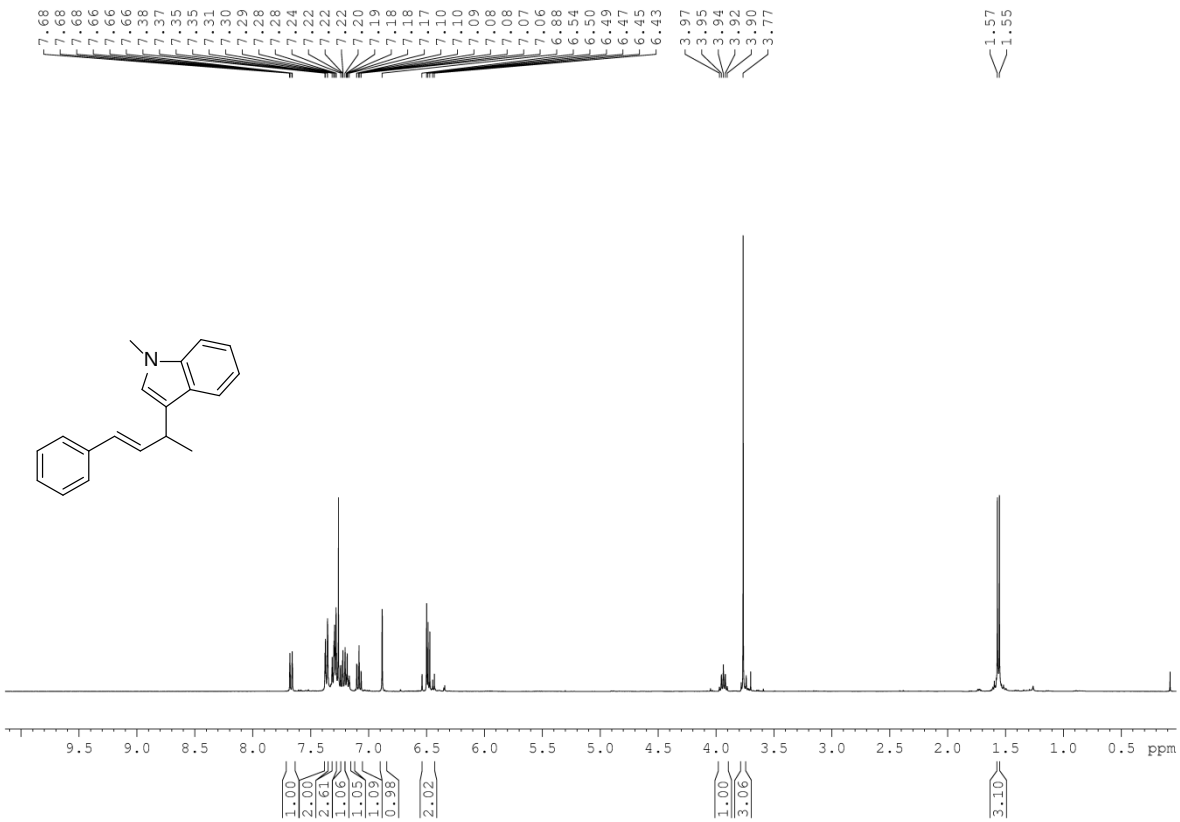
^{1}H NMR ($CDCl_3$, 400 MHz) of **19a**:



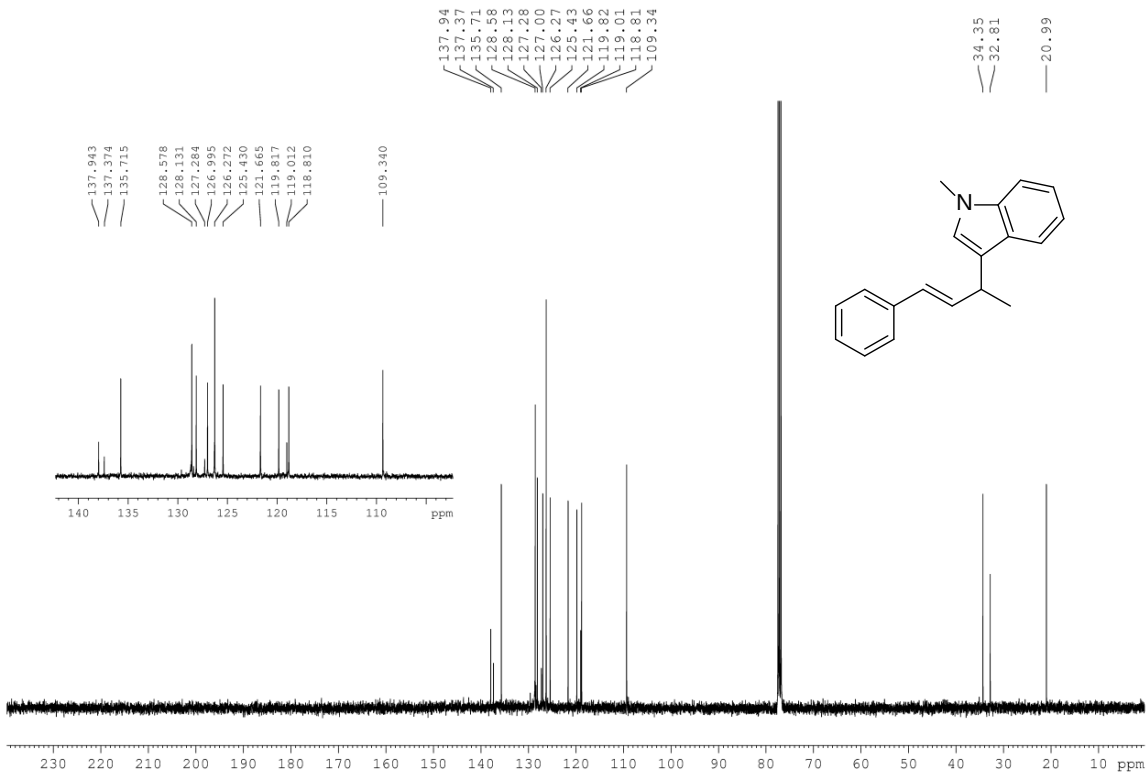
^{13}C NMR ($CDCl_3$, 100 MHz) of **19a**:



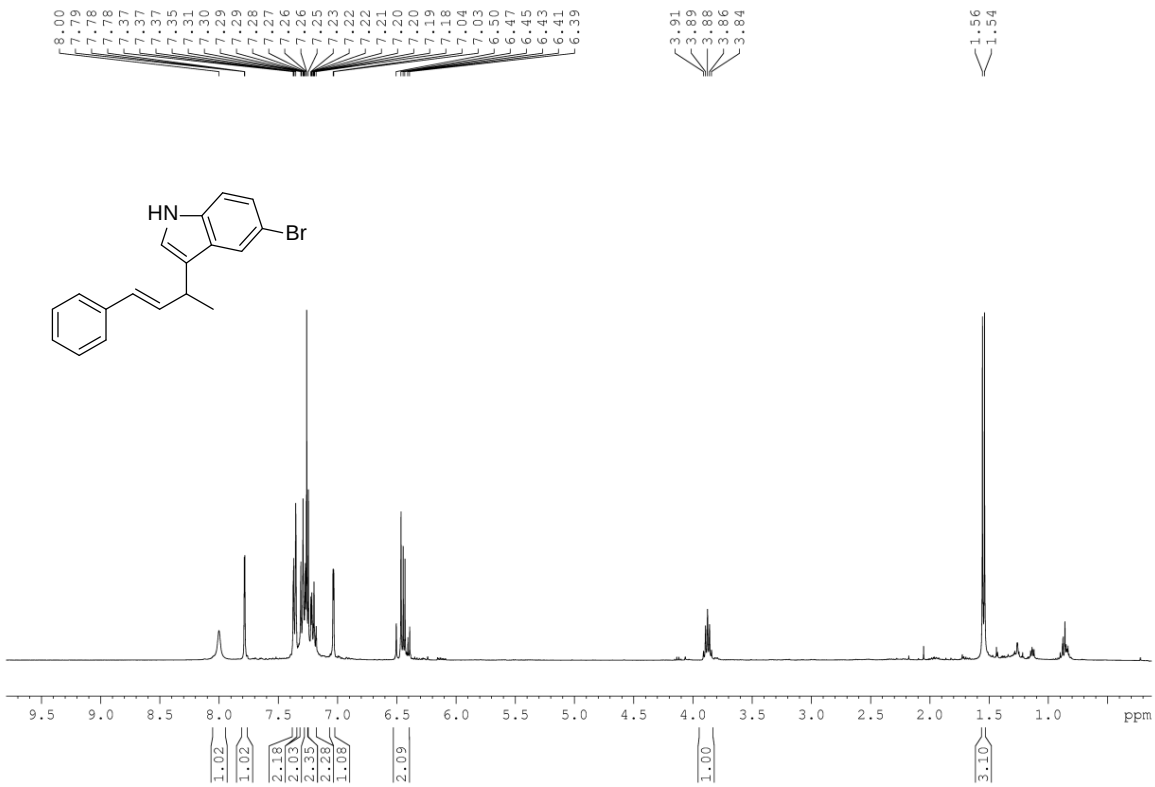
^{1}H NMR ($CDCl_3$, 400 MHz) of **19b**:



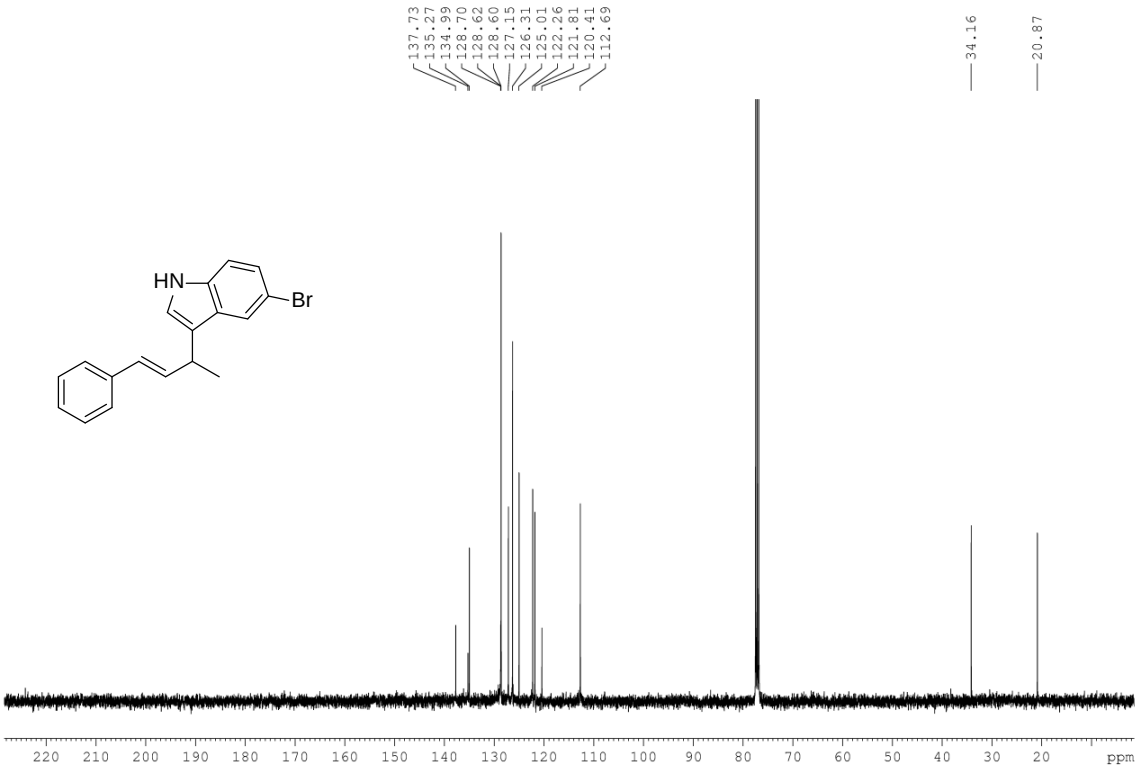
^{13}C NMR ($CDCl_3$, 100 MHz) of **19b**:



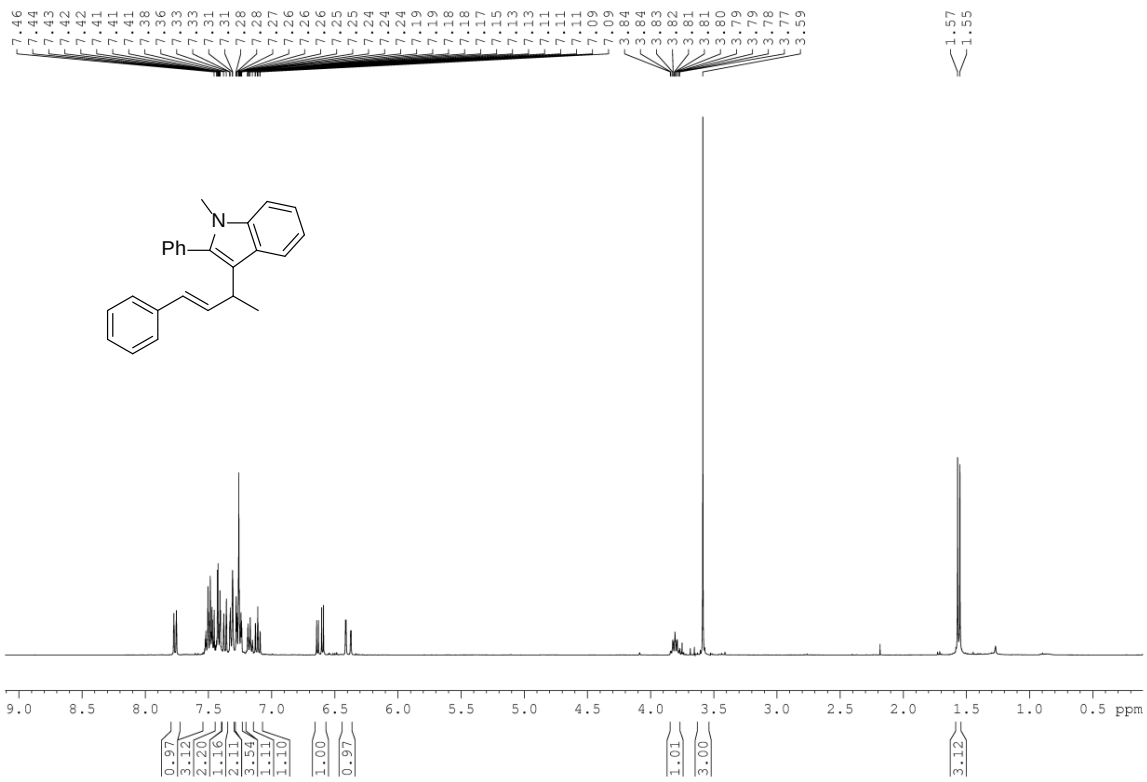
^{1}H NMR ($CDCl_3$, 400 MHz) of **19c**:



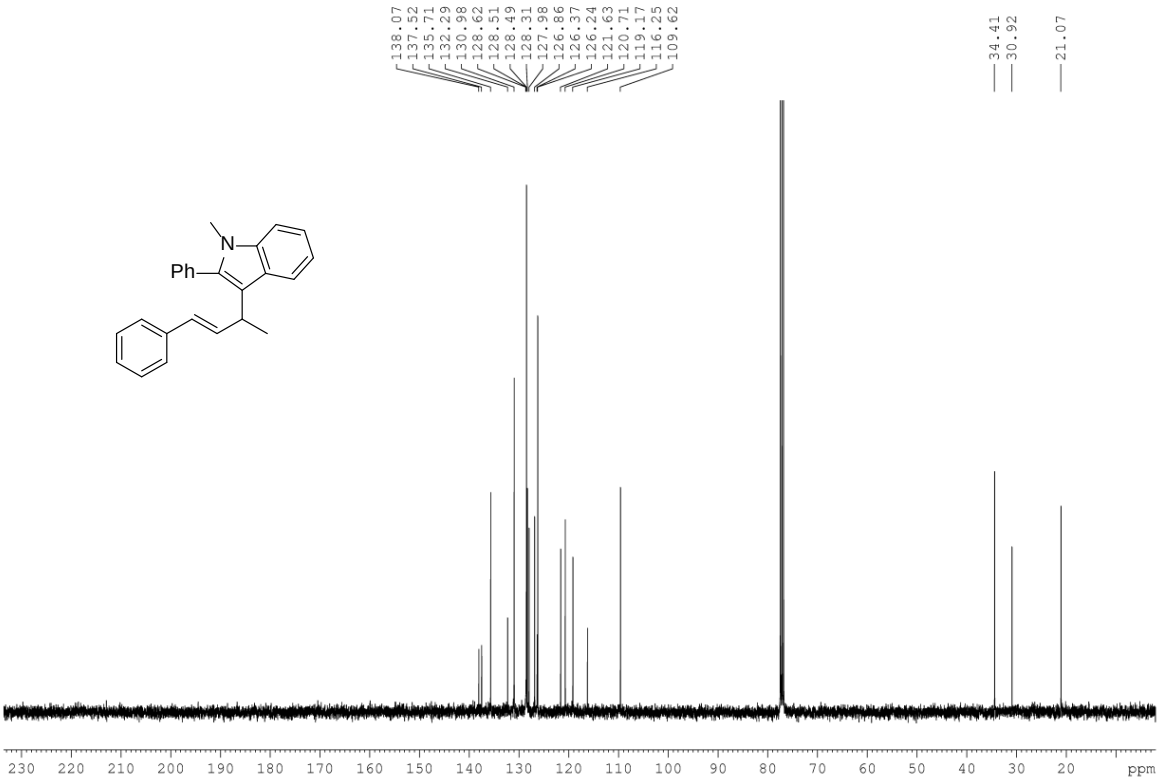
^{13}C NMR ($CDCl_3$, 100 MHz) of **19c**:



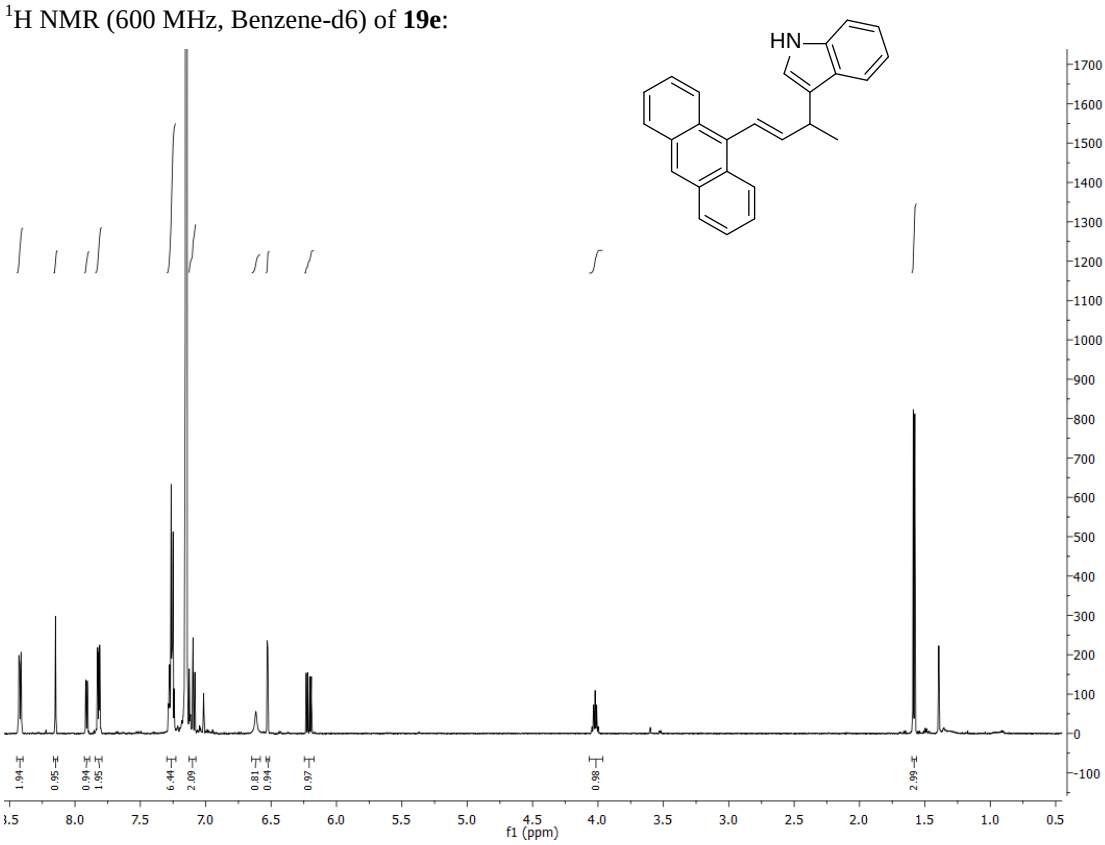
^{1}H NMR ($CDCl_3$, 400 MHz) of **19d**:



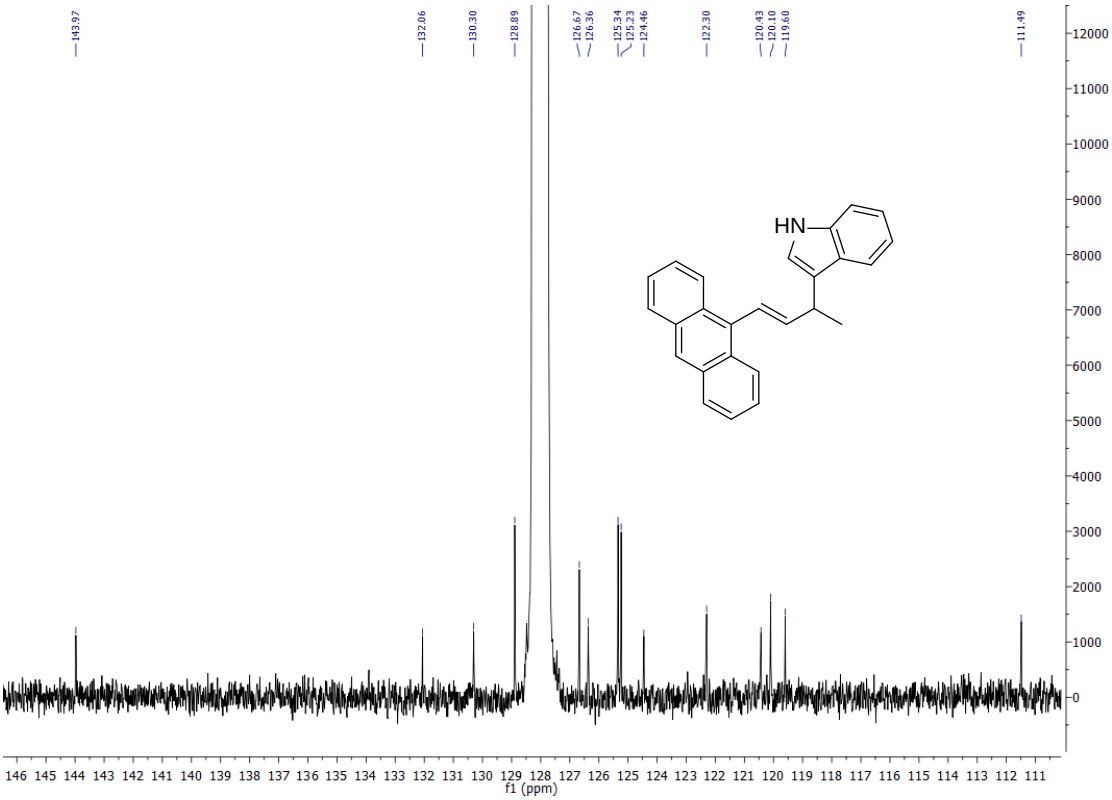
^{13}C NMR ($CDCl_3$, 100 MHz) of **19d**:



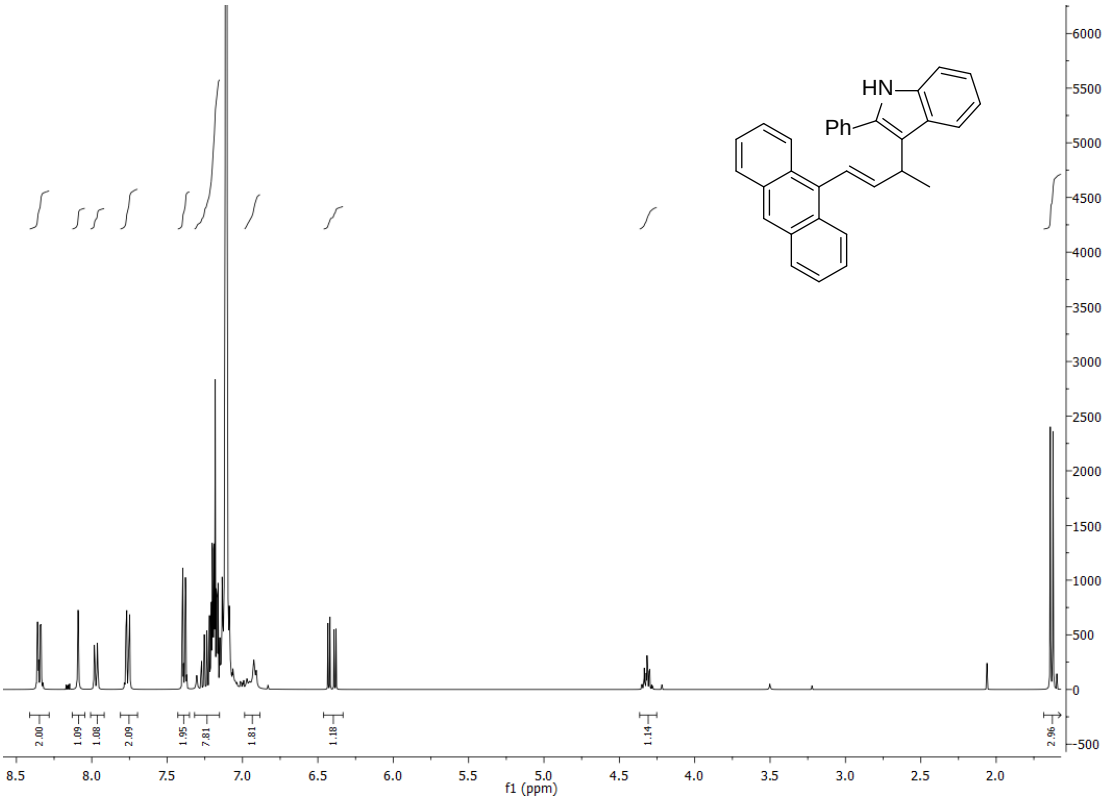
^{1}H NMR (600 MHz, Benzene-d6) of **19e**:



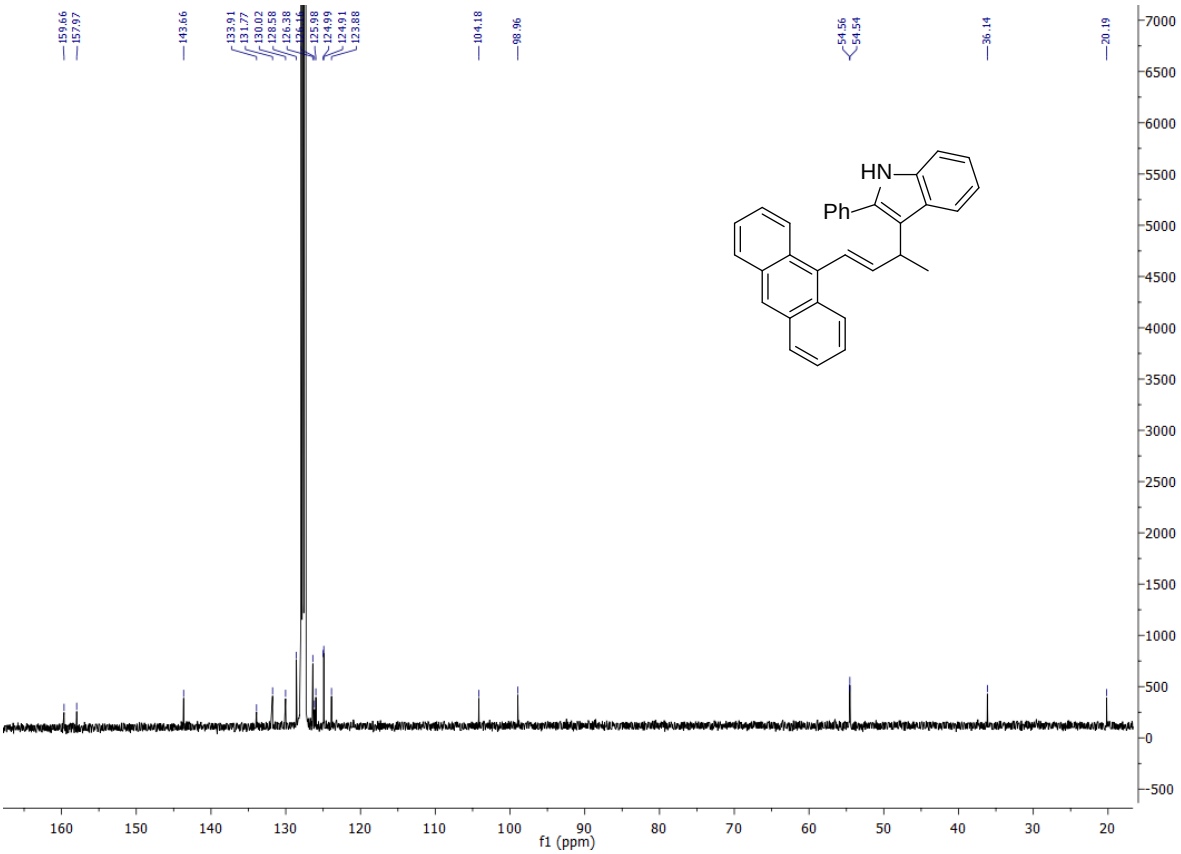
^{13}C NMR (126 MHz, C_6D_6) of **19e**:



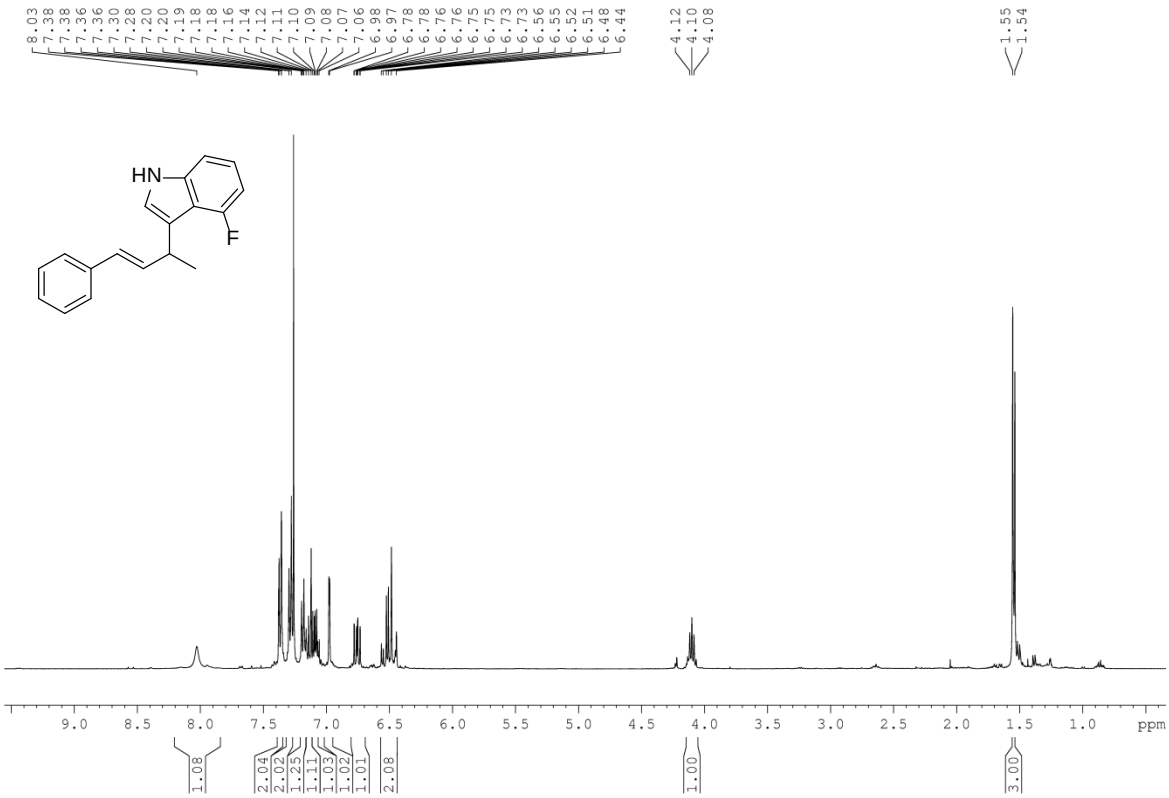
^{1}H NMR ($CDCl_3$, 400 MHz) of **19f**:



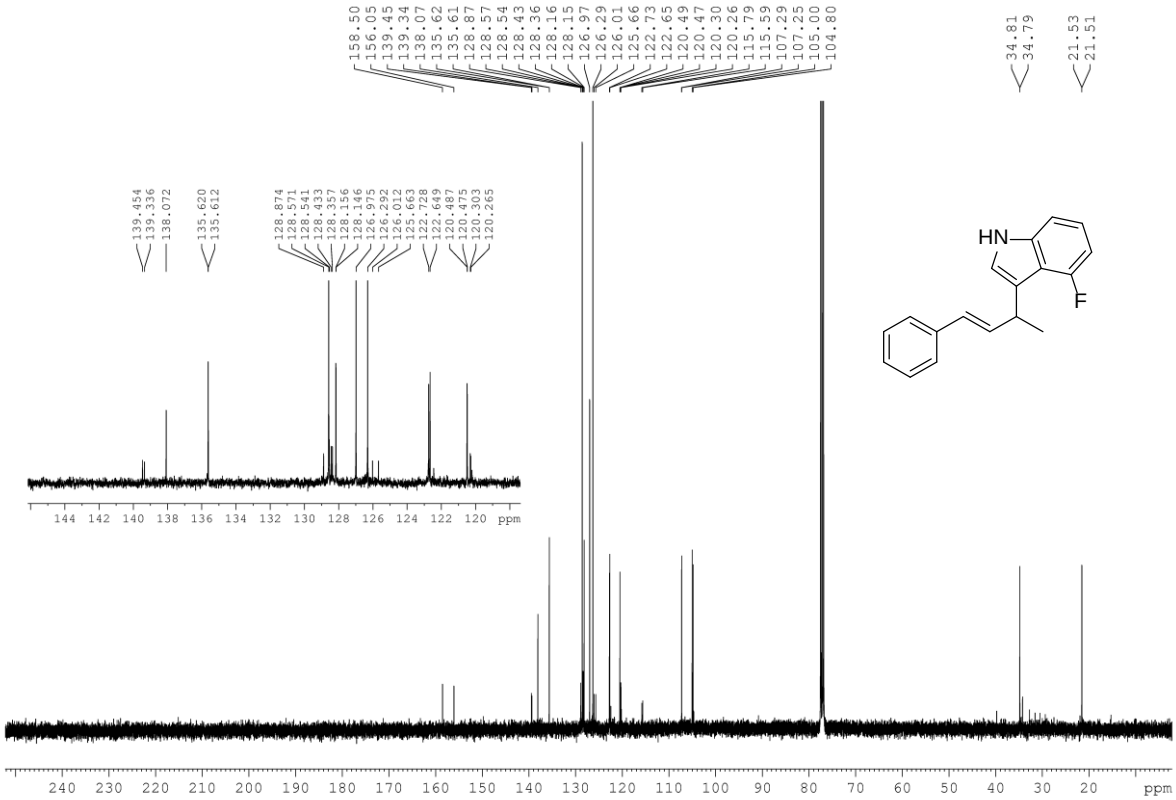
^{13}C NMR ($CDCl_3$, 100 MHz) of **19f**:



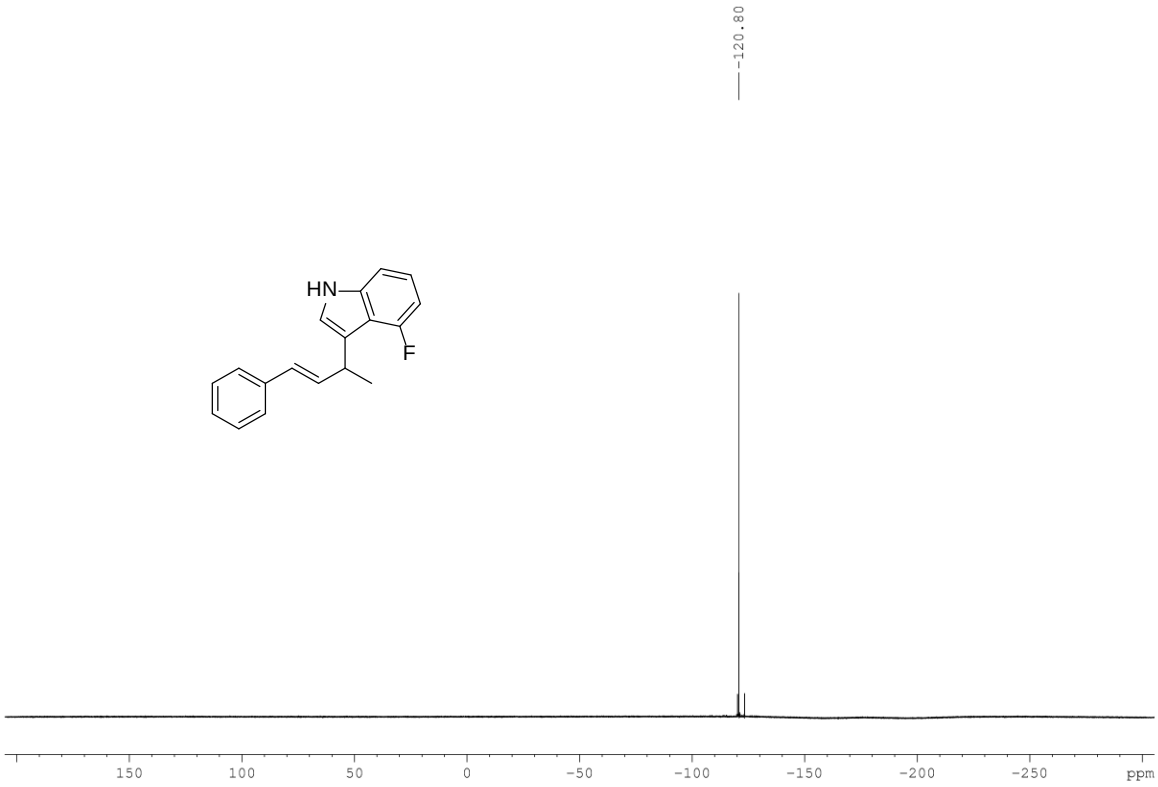
^{1}H NMR ($CDCl_3$, 400 MHz) of **19g**:



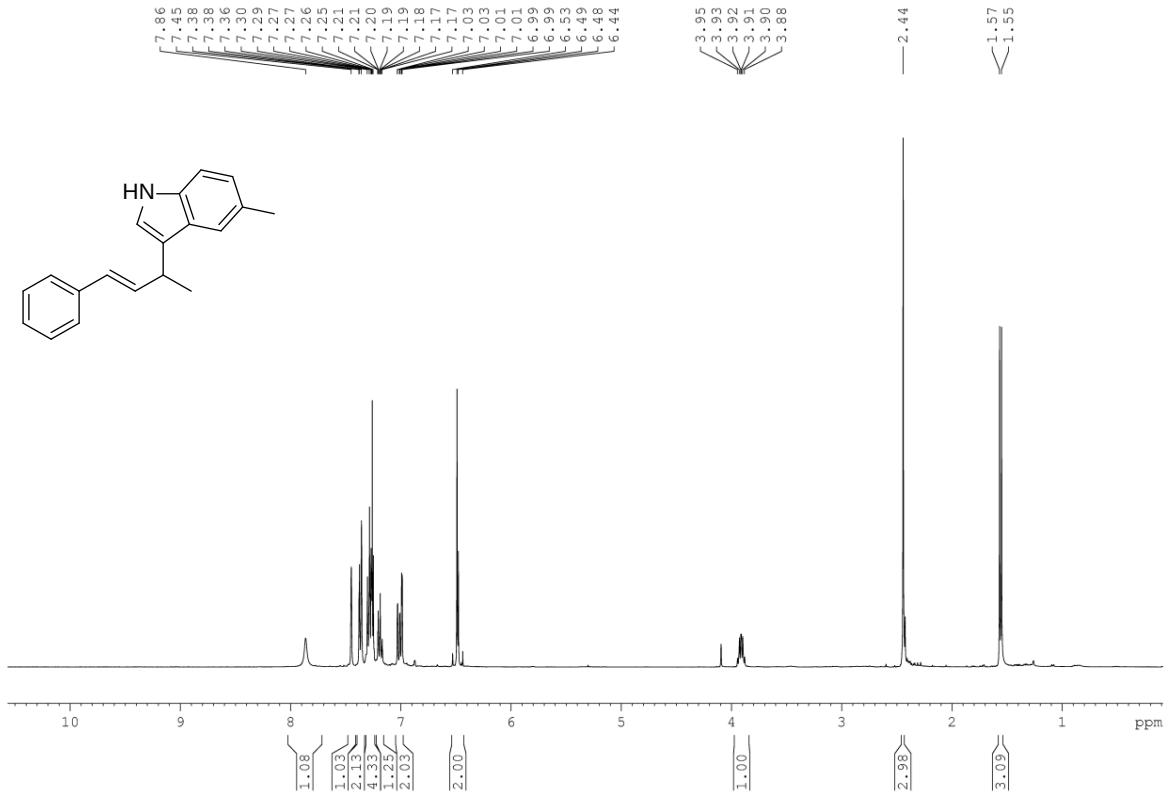
^{13}C NMR ($CDCl_3$, 100 MHz) of **19g**:



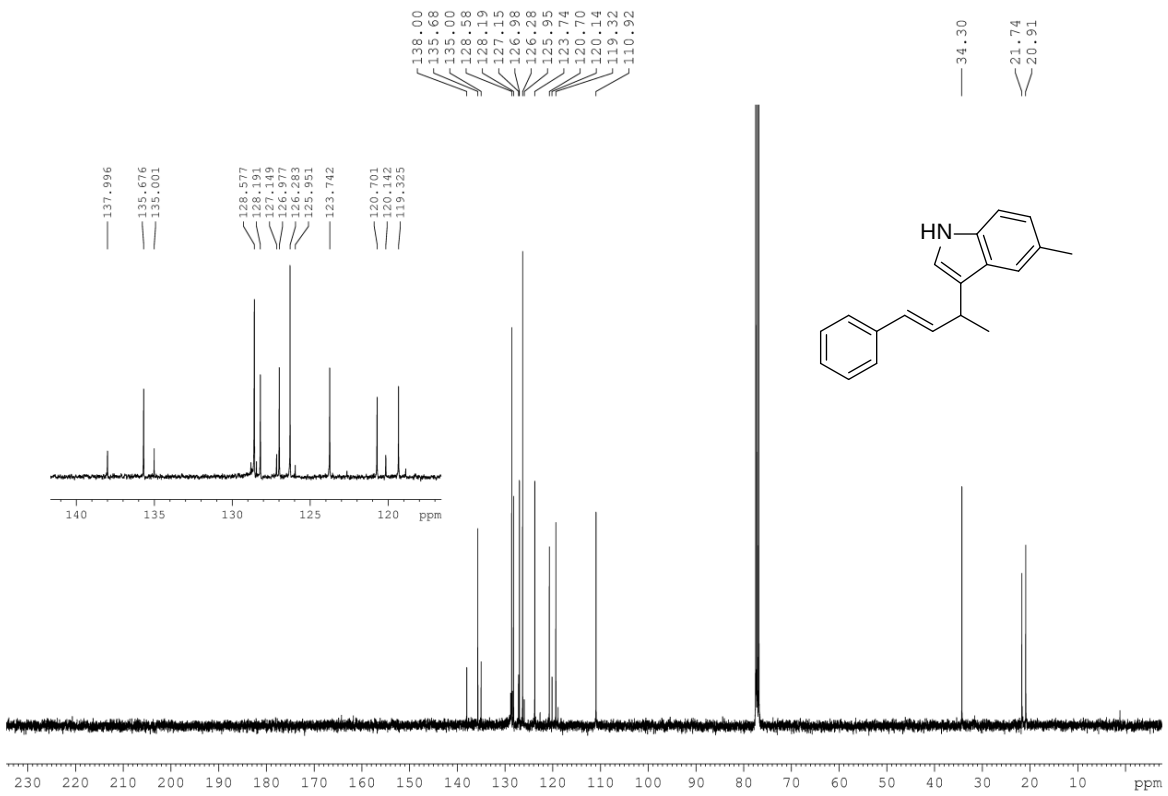
^{19}F NMR ($CDCl_3$, 282 MHz) of **19g**:



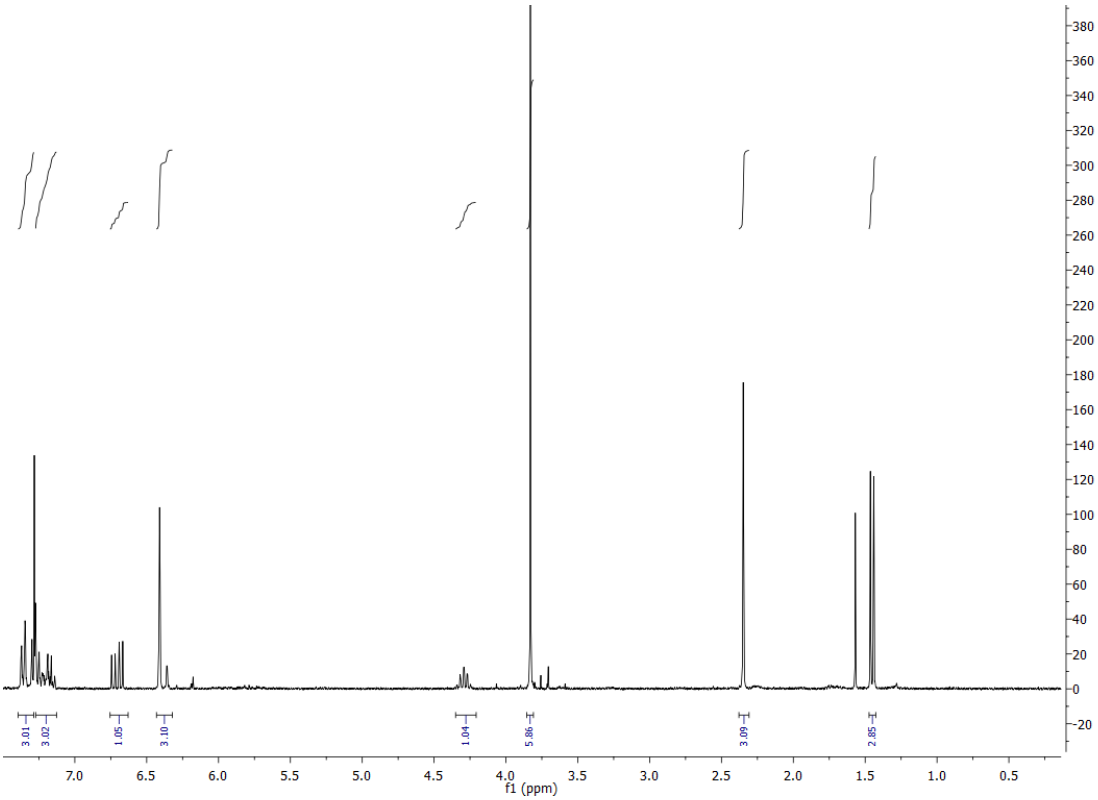
^{1}H NMR ($CDCl_3$, 400 MHz) of **19h**:



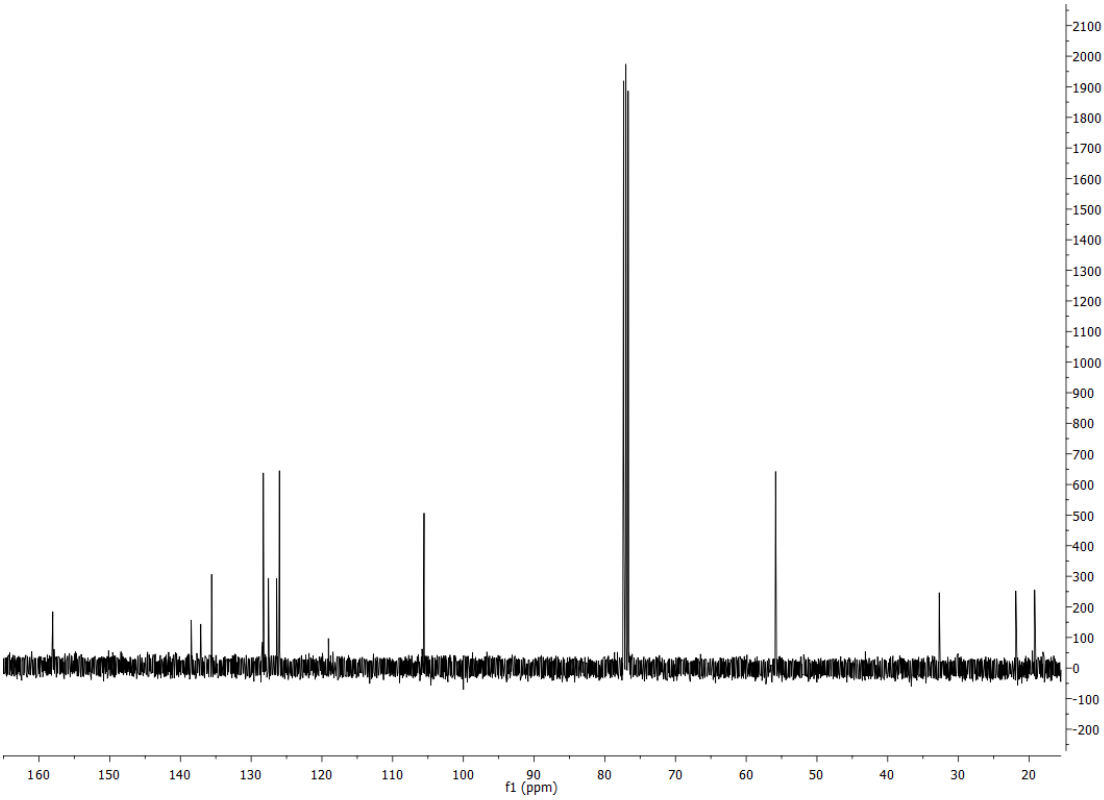
^{13}C NMR ($CDCl_3$, 100 MHz) of **19h**:



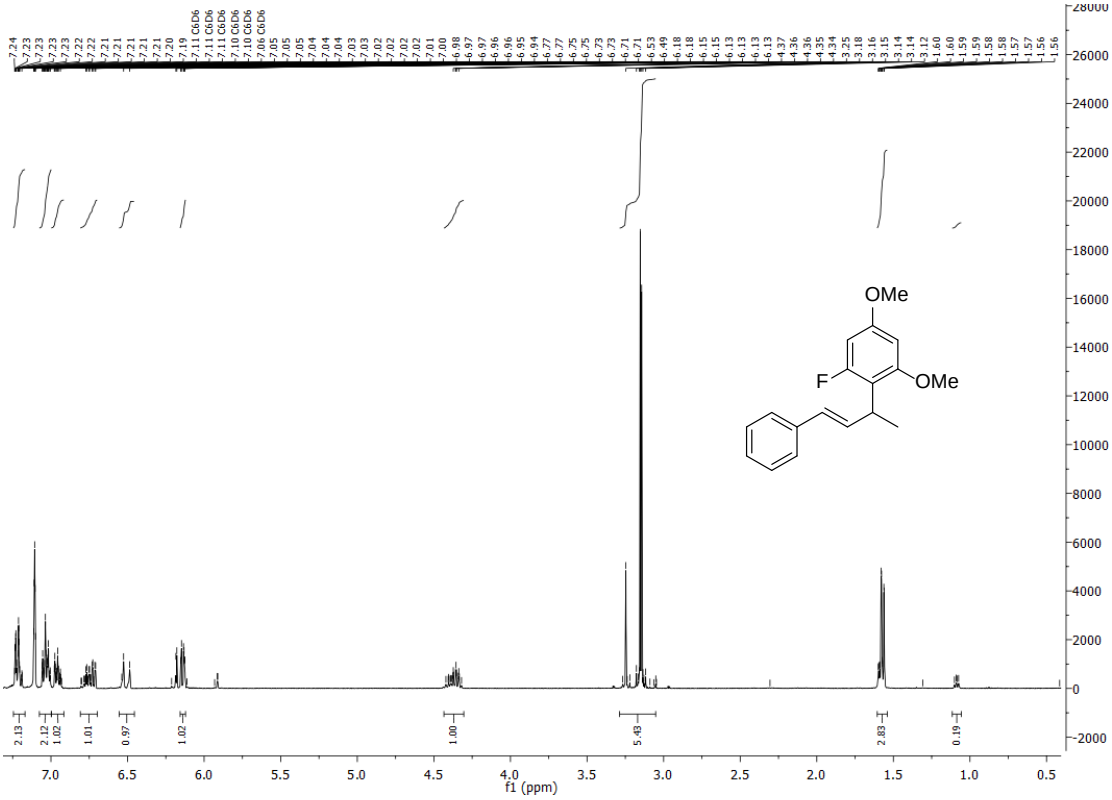
^{1}H NMR (300 MHz, $CDCl_3$,) of **19i**:



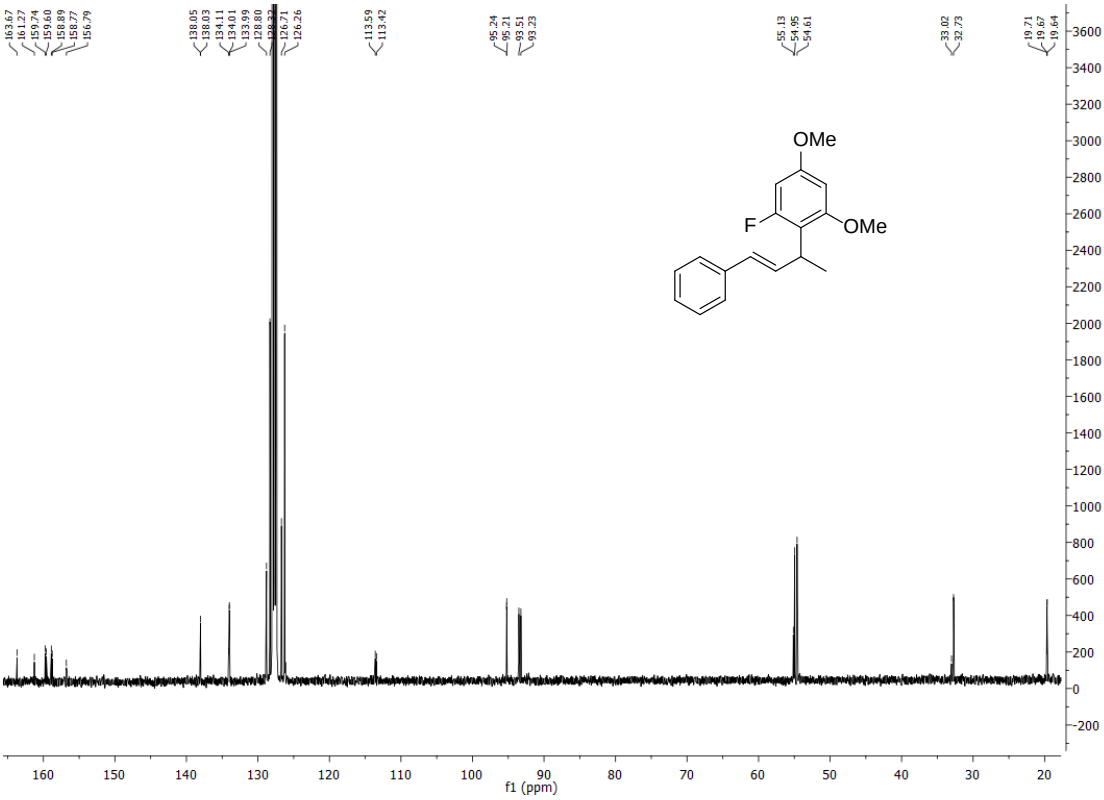
^{13}C NMR ($CDCl_3$, 100 MHz) of **19i**:



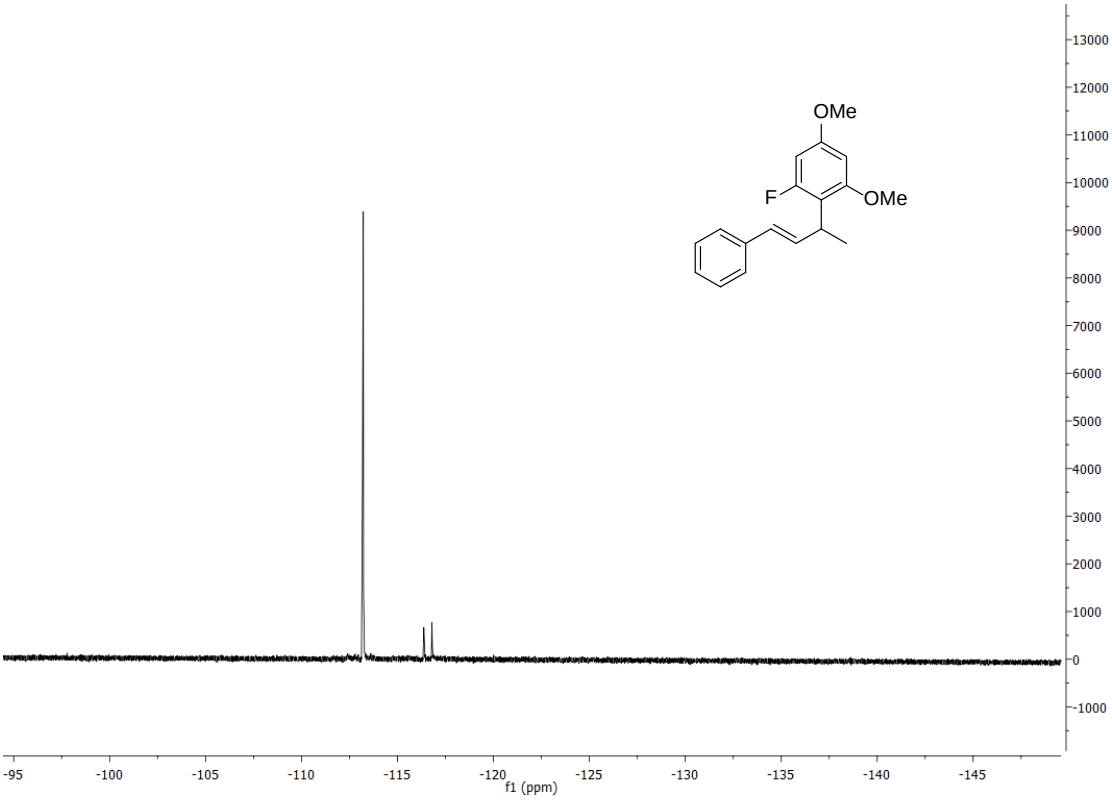
^{1}H NMR ($CDCl_3$, 400 MHz) of **19j** (mixture of regioisomers):



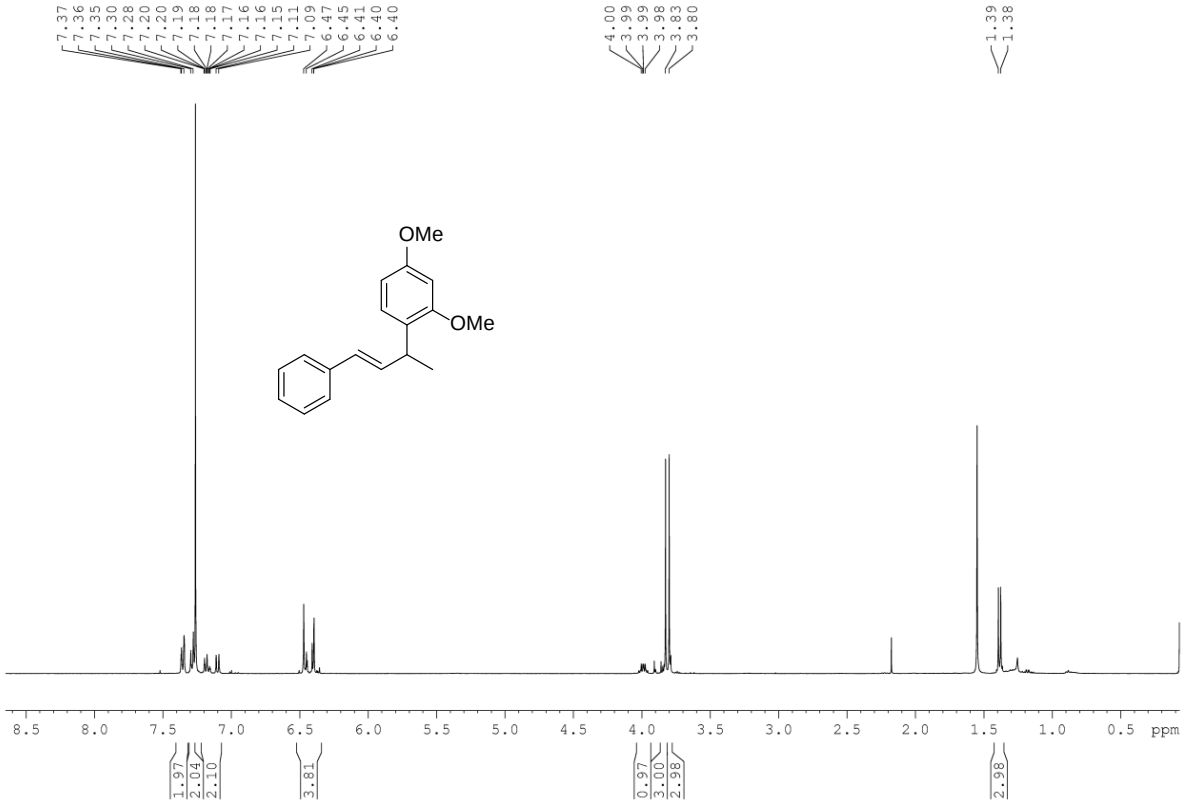
^{13}C NMR ($CDCl_3$, 100 MHz) of **19j** (mixture of regioisomers):



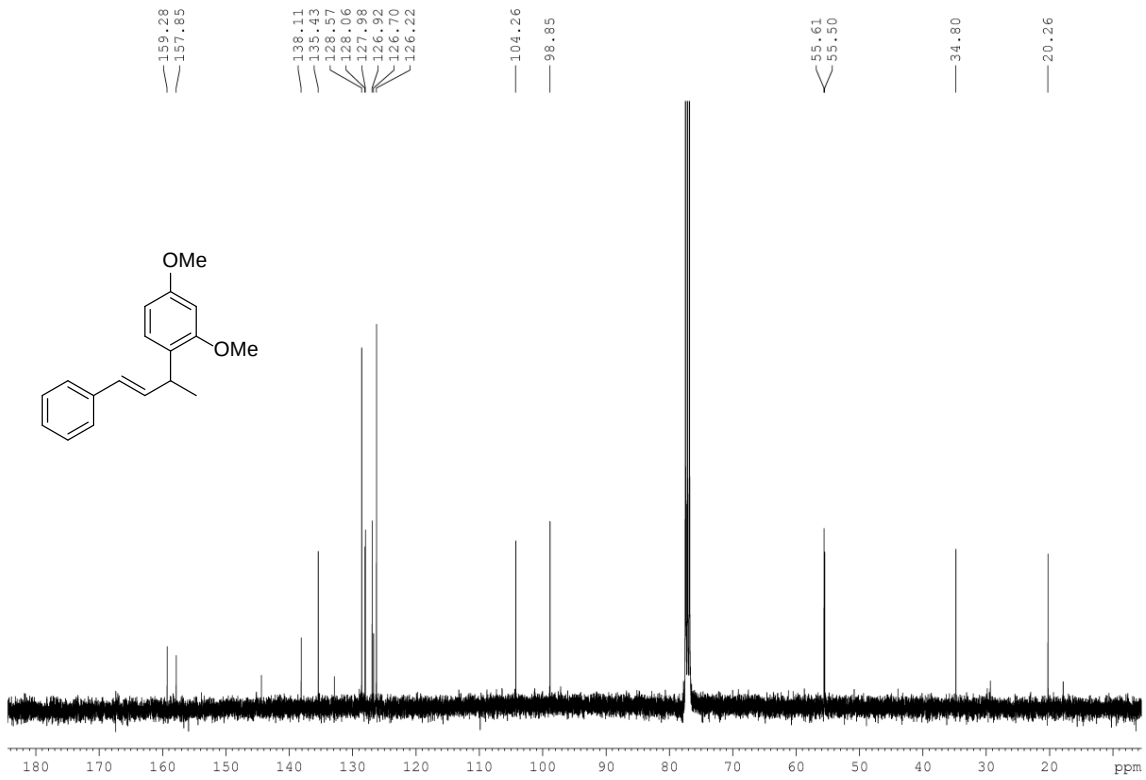
^{19}F NMR ($CDCl_3$, 282 MHz) of **19j** (mixture of regioisomers):



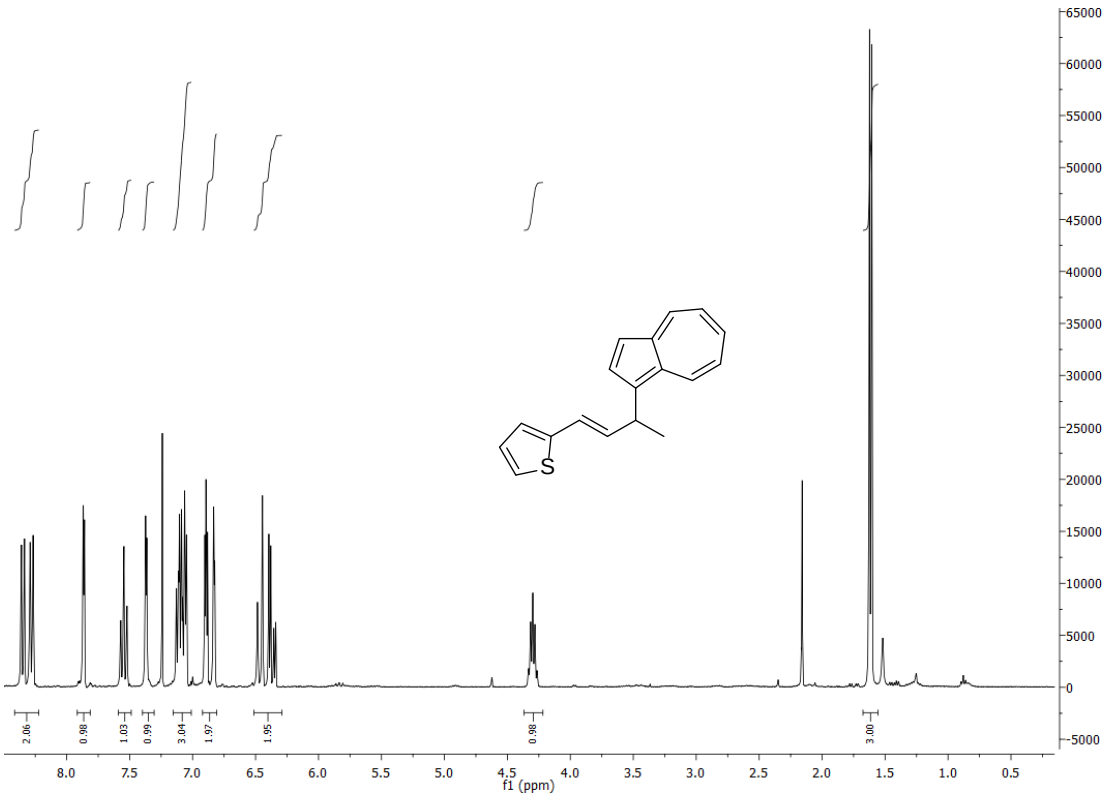
^{1}H NMR ($CDCl_3$, 400 MHz) of **19k**:



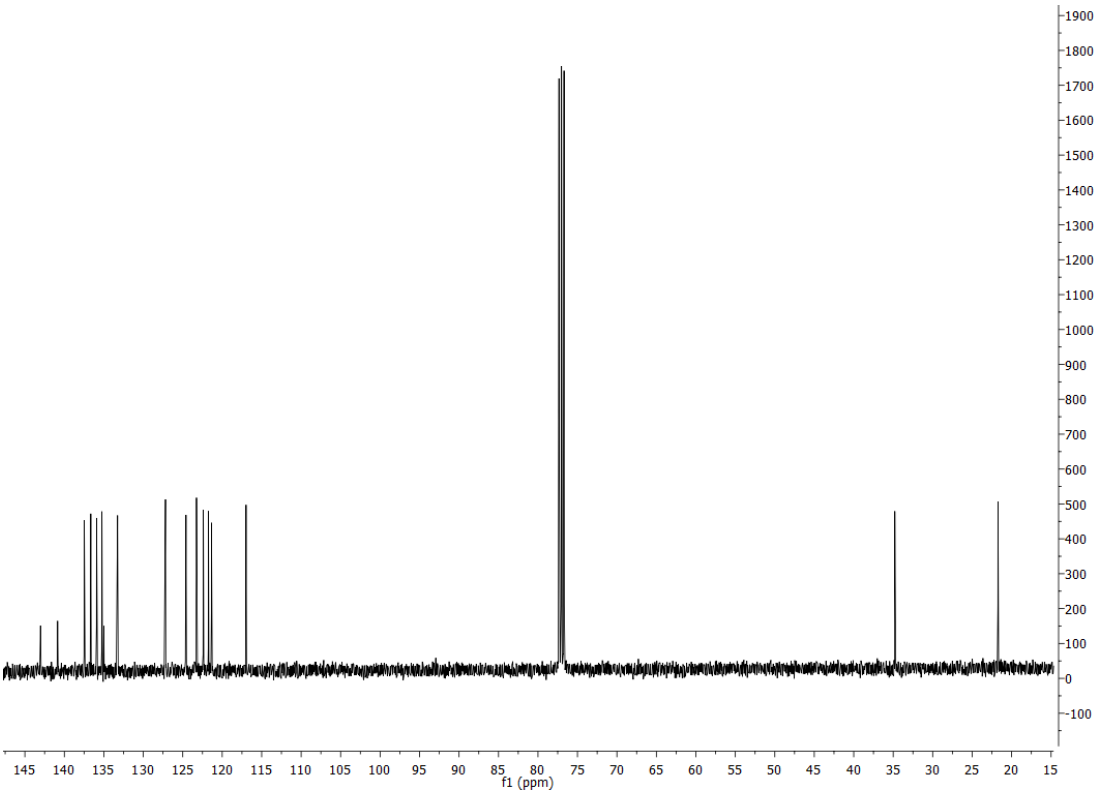
^{13}C NMR ($CDCl_3$, 100 MHz) of **19k**:



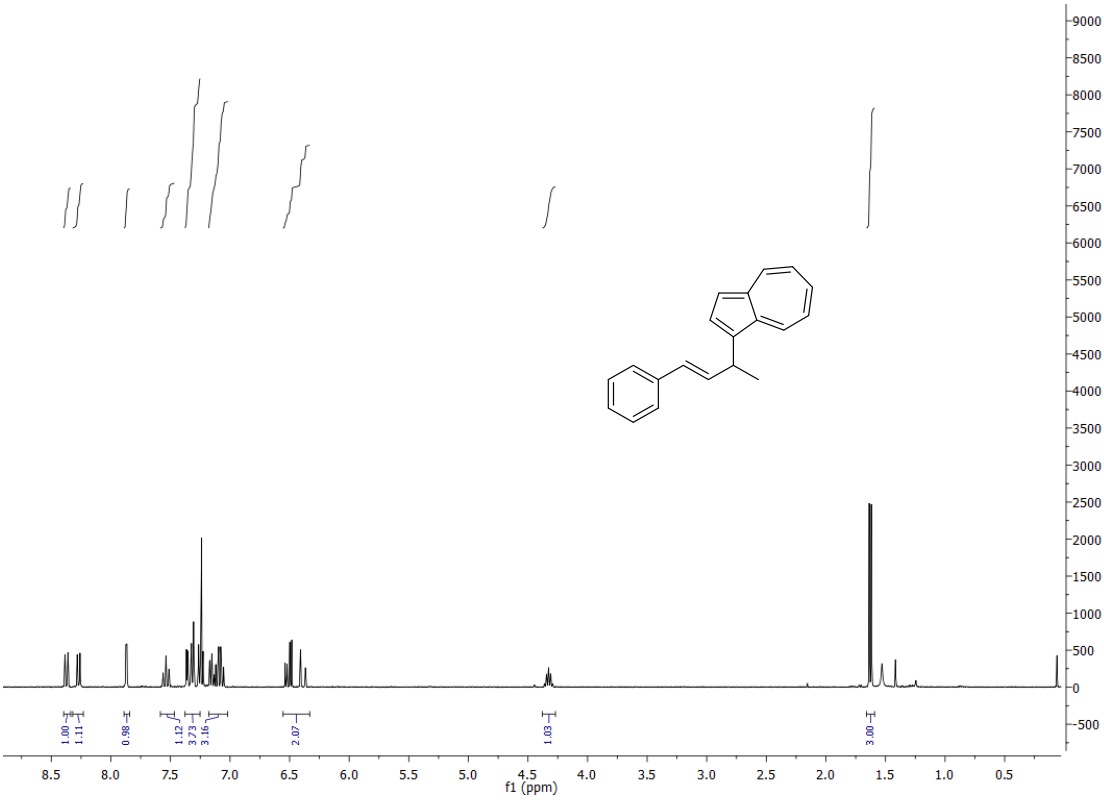
^{1}H NMR ($CDCl_3$, 400 MHz) of **19l**:



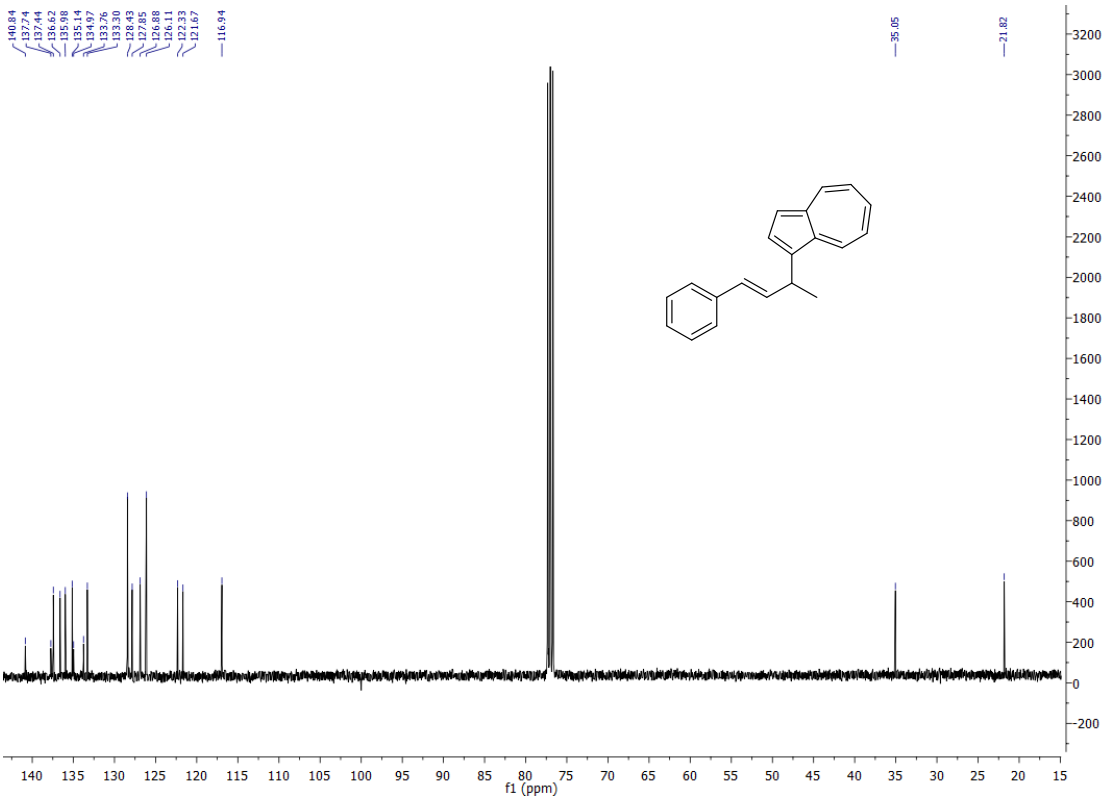
^{13}C NMR ($CDCl_3$, 100 MHz) of **19l**:



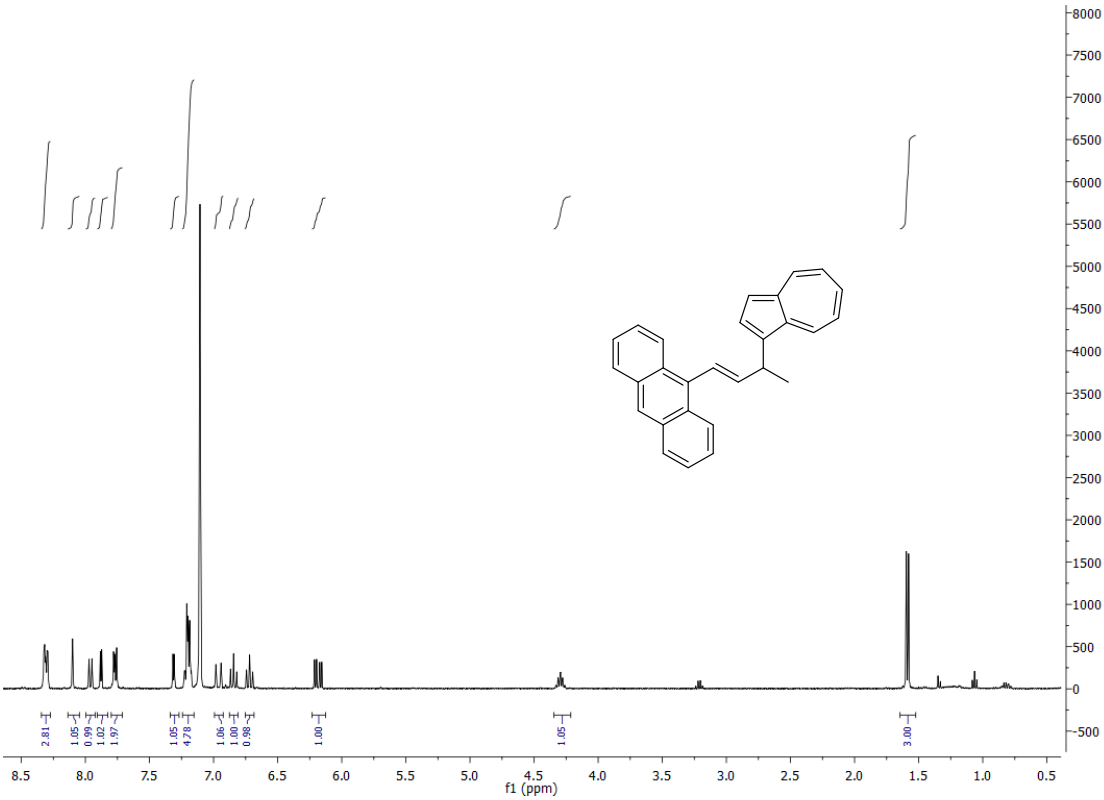
^{1}H NMR ($CDCl_3$, 400 MHz) of **19n**:



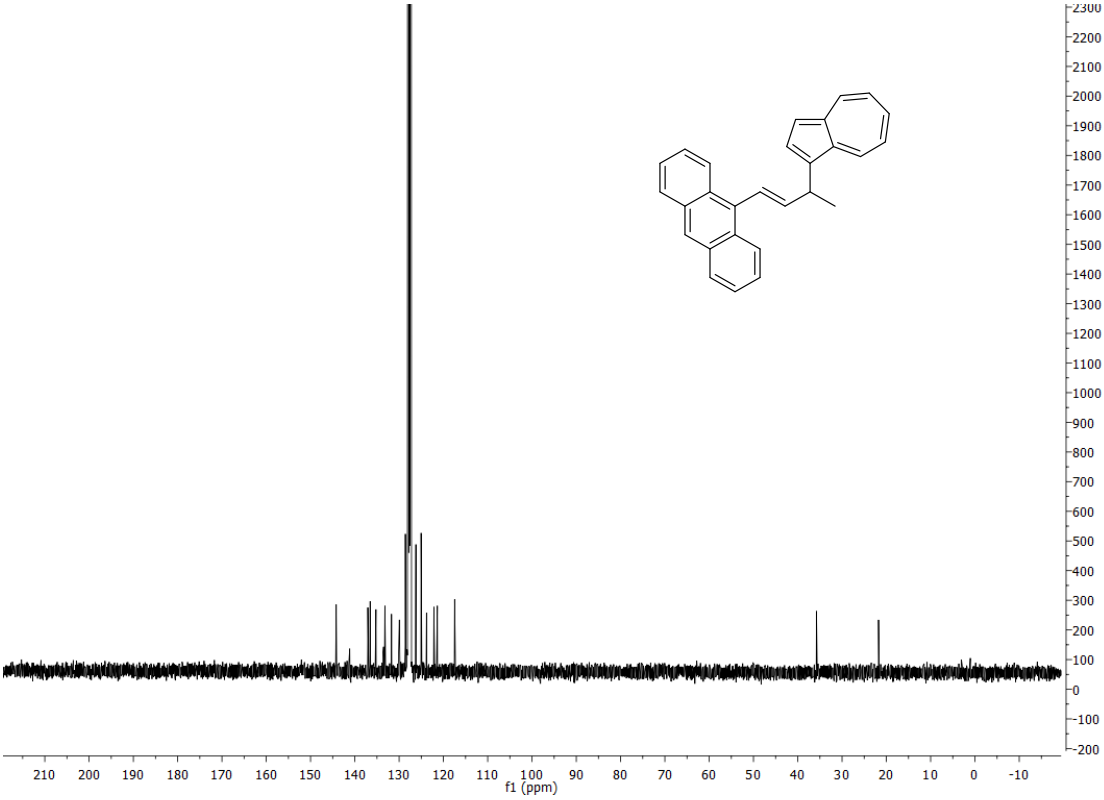
^{13}C NMR ($CDCl_3$, 100 MHz) of **19n**:



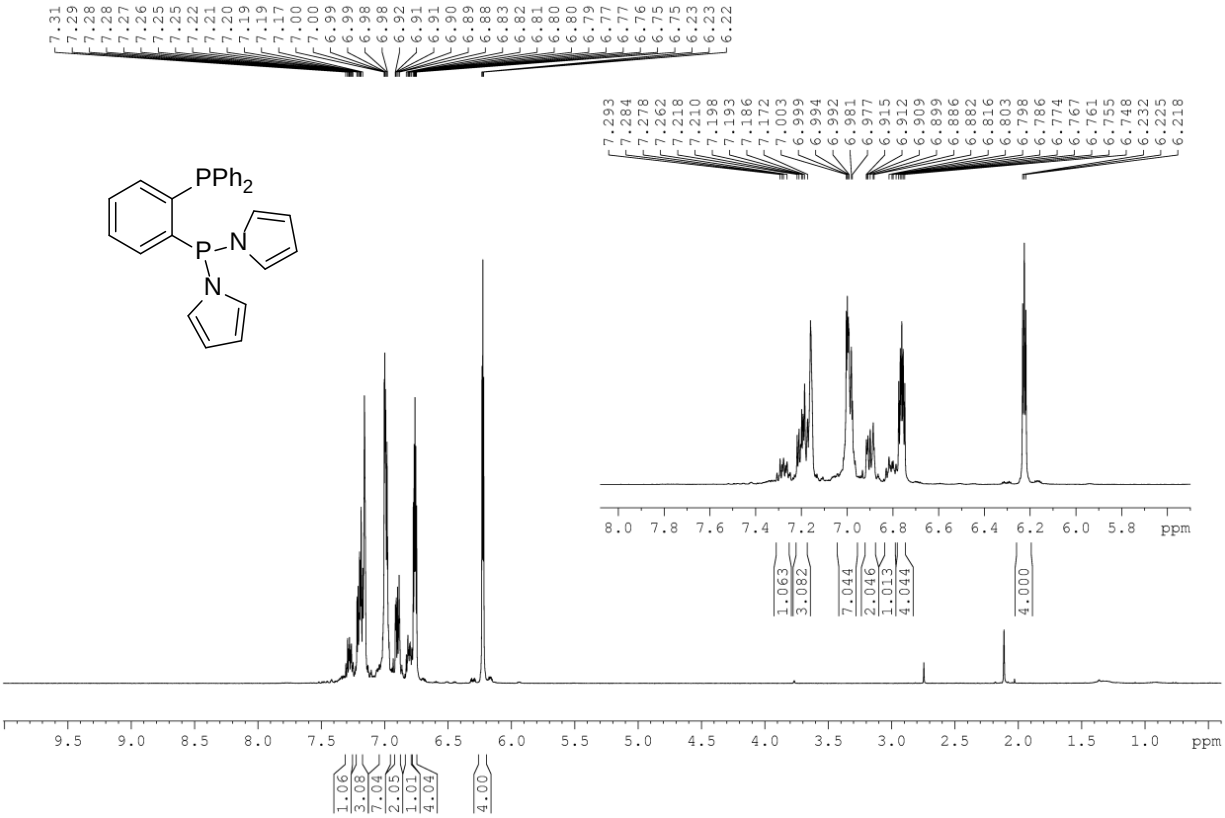
^{1}H NMR (400 MHz, C_6D_6) of **19m**:



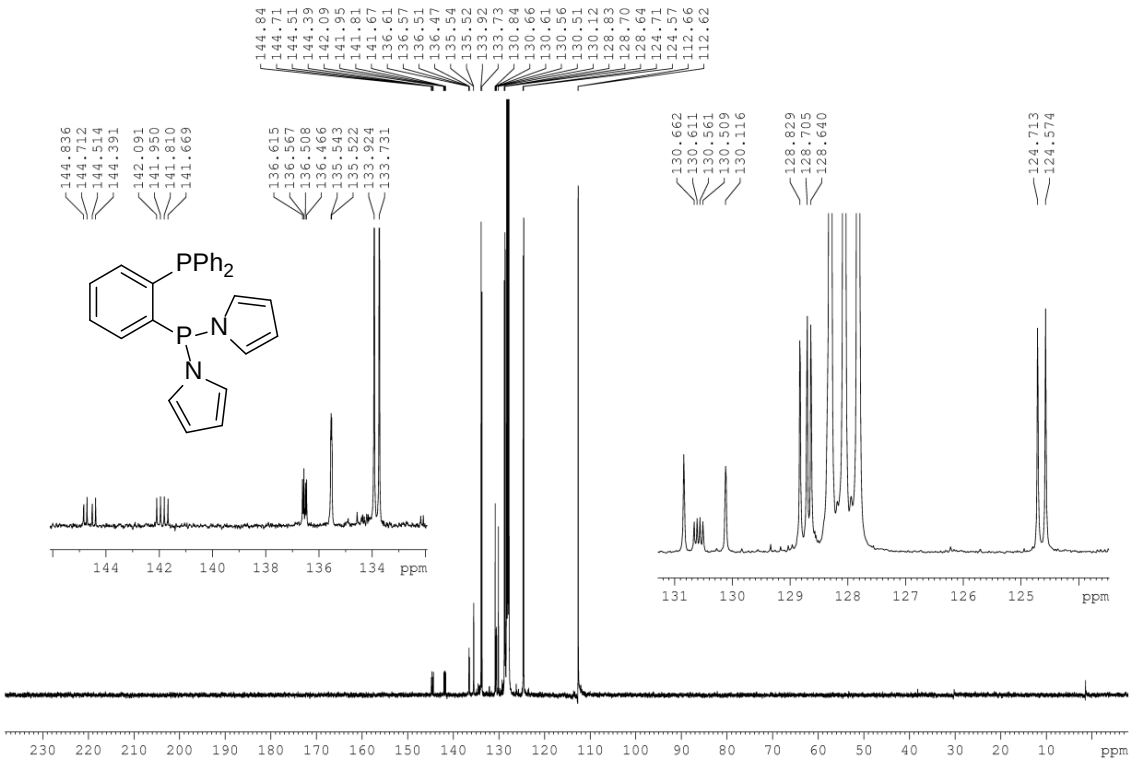
^{13}C NMR (101 MHz, C_6D_6) of **19m**:



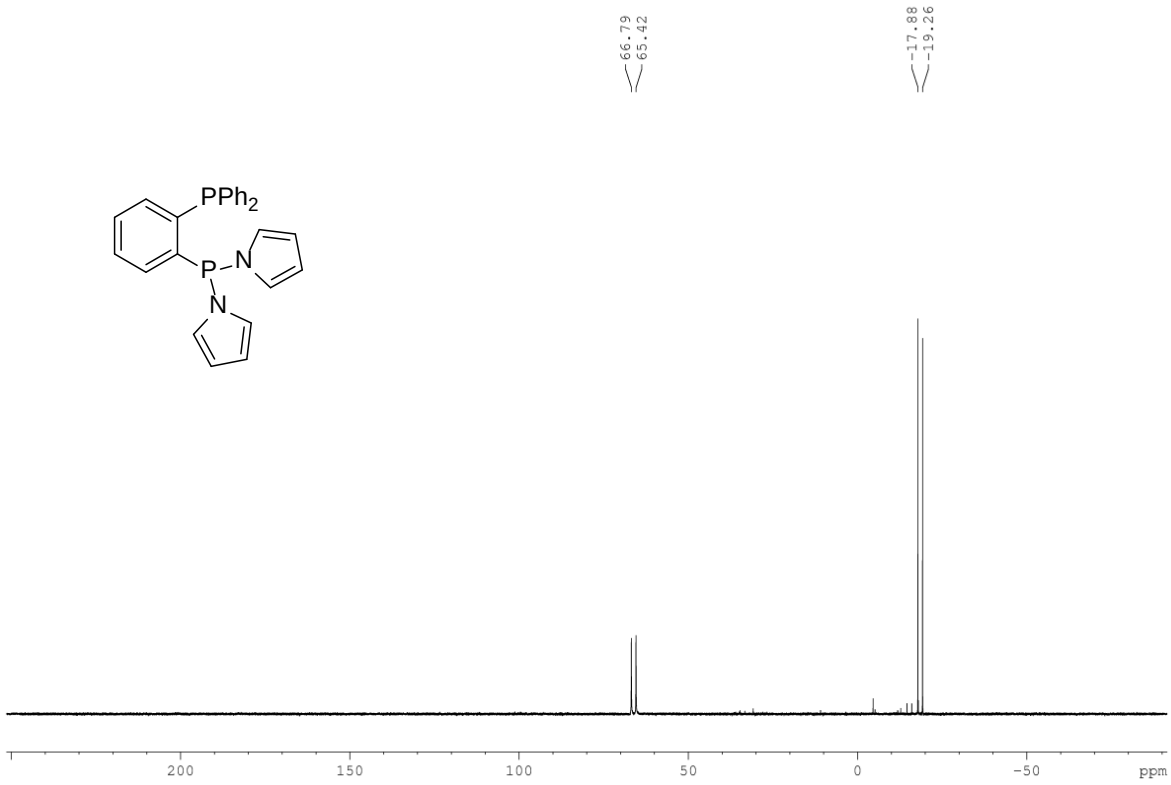
^{1}H NMR (C_6D_6, 300 MHz) of **20**:



^{13}C NMR (C_6D_6, 100 Mz) of **20**:

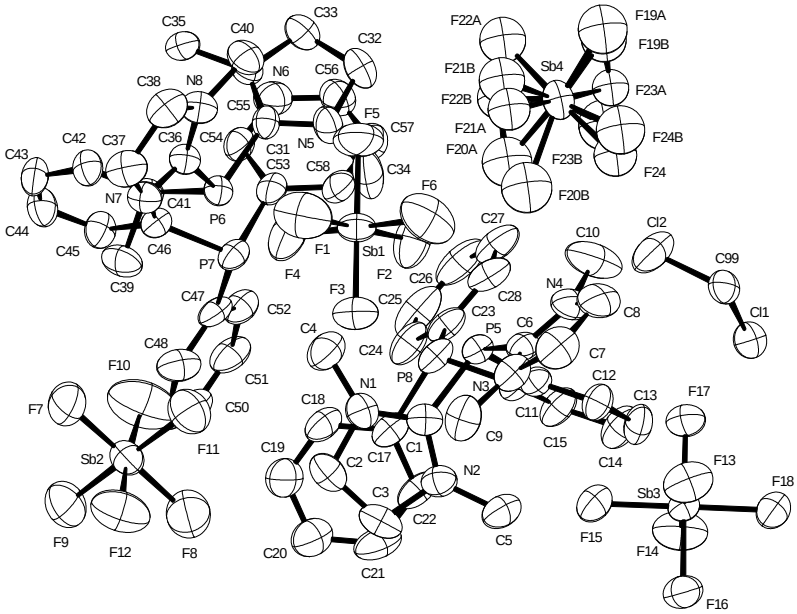


^{31}P NMR (C_6D_6, 121 MHz) of **20**:



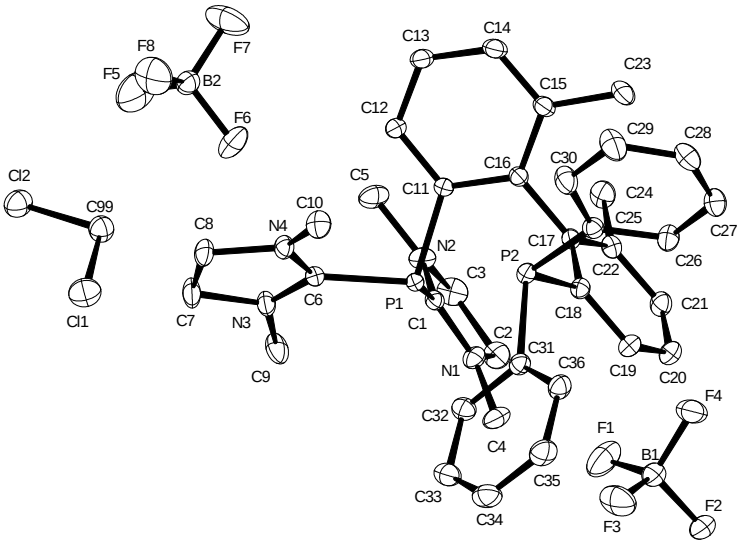
X-ray Structures

Compound **1**



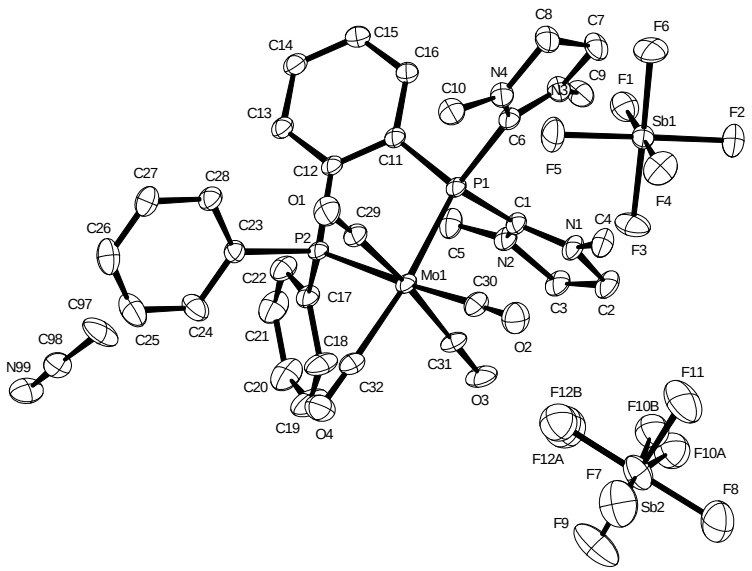
Empirical formula	$C_{28}H_{34}F_{12}N_4P_2Sb_2 \cdot 0.25\ CH_2Cl_2$	
Color	colorless	
Formula weight	981.26 $g \cdot mol^{-1}$	
Temperature	150 K	
Wavelength	1.54178 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 15.3374(6) Å	α= 90°.
	b = 37.0863(14) Å	β= 104.8921(17)°.
	c = 13.4231(5) Å	γ = 90°.
Volume	7378.7(5) $Å^3$	
Z	8	
Density (calculated)	1.767 $Mg \cdot m^{-3}$	
Absorption coefficient	13.564 mm^{-1}	
F(000)	3844 e	
Crystal size	0.20 x 0.11 x 0.03 mm^3	
□range for data collection	2.383 to 65.082°.	
Index ranges	$-18 \le h \le 17$, $-43 \le k \le 43$, $-15 \le l \le 15$	
Reflections collected	172322	
Independent reflections	12440 [R_{int} = 0.0844]	
Reflections with I>2 σ (I)	10497	
Completeness to θ = 67.679°	93.1 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.68 and 0.08	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12440 / 0 / 895	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2 σ (I)]	R_1 = 0.0724	wR^2 = 0.1879
R indices (all data)	R_1 = 0.0840	wR^2 = 0.1972
Extinction coefficient	0.00034(3)	
Largest diff. peak and hole	1.8 and -1.6 e $\cdot Å^{-3}$	

Compound **2**



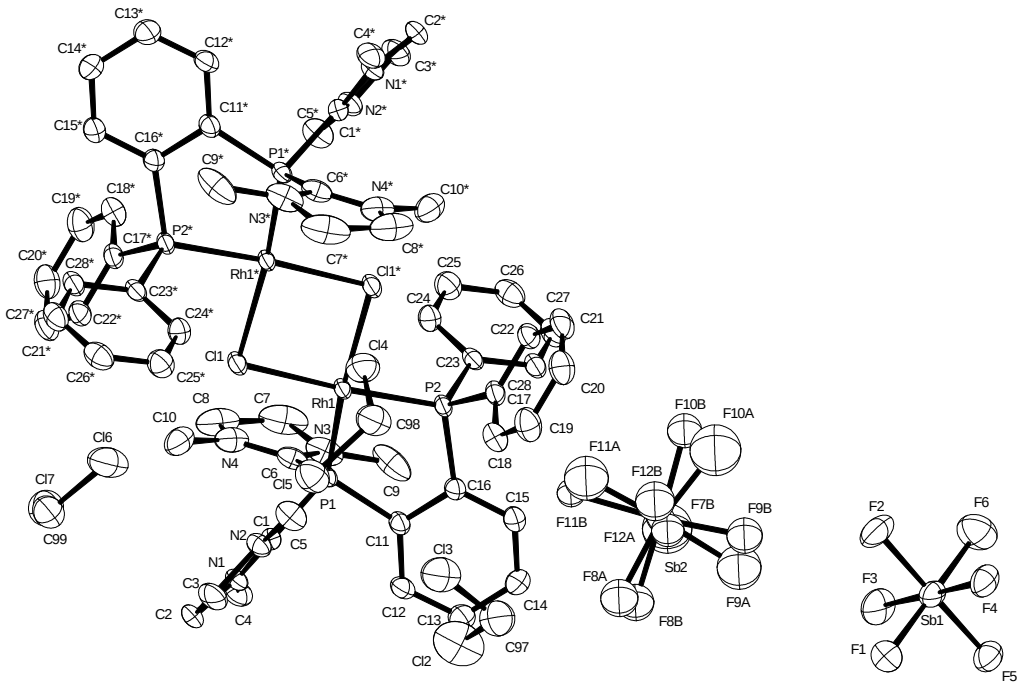
Empirical formula	$C_{37}H_{44}B_2Cl_2F_8N_4P_2$	
Color	yellow	
Formula weight	851.22 g · mol^{-1}	
Temperature	100.15 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 19.5245(8) Å	α= 90°.
	b = 12.1720(11) Å	β= 102.298(4)°.
	c = 17.6079(10) Å	γ = 90°.
Volume	4088.5(5) Å^3	
Z	4	
Density (calculated)	1.383 Mg · m^{-3}	
Absorption coefficient	0.306 mm^{-1}	
F(000)	1760 e	
Crystal size	0.18 x 0.18 x 0.17 mm^3	
θ range for data collection	2.713 to 33.139°.	
Index ranges	$-30 \leq h \leq 30$, $-18 \leq k \leq 18$, $-27 \leq l \leq 27$	
Reflections collected	123046	
Independent reflections	15544 [R_{int} = 0.0289]	
Reflections with I>2 σ (I)	13476	
Completeness to θ = 25.242°	99.6 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.75 and 0.68	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15544 / 0 / 502	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2 σ (I)]	R_1 = 0.0342	wR^2 = 0.0892
R indices (all data)	R_1 = 0.0420	wR^2 = 0.0949
Largest diff. peak and hole	0.6 and -0.5 e · Å^{-3}	

Compound **8:**



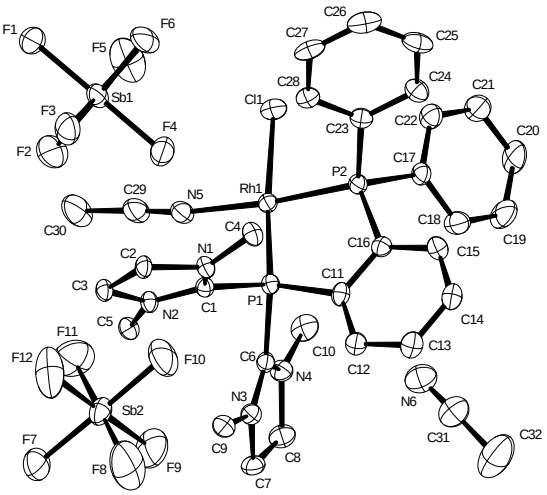
Empirical formula	$C_{33}H_{35.50}F_{12}MoN_{4.50}O_4P_2Sb_2$	
Color	yellow	
Formula weight	1188.54 g · mol-1	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	TRICLINIC	
Space group	**$P^{-}1$, (no. 2)**	
Unit cell dimensions	a = 10.5620(5) Å	α = 99.497(8)°.
	b = 14.8442(13) Å	β = 92.181(6)°.
	c = 14.9641(14) Å	γ = 92.074(6)°.
Volume	2310.2(3) Å3	
Z	2	
Density (calculated)	1.709 mg · m-3	
Absorption coefficient	1.584 mm-1	
F(000)	1158 e	
Crystal size	0.15 x 0.08 x 0.03 mm3	
θ range for data collection	2.633 to 32.031°.	
Index ranges	15 ≤ h ≤ -15, 21 ≤ k ≤ -22, 22 ≤ l ≤ 0	
Reflections collected	53813	
Independent reflections	15951 [Rint = 0.0520]	
Reflections with I>2σ(I)	14303	
Completeness to θ = 25.242°	99.20%	
Absorption correction	Gaussian	
Max. and min. transmission	0.75 and 0.44	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	15951 / 0 / 544	
Goodness-of-fit on F2	1.042	
Final R indices [I>2 σ(I)]	R1 = 0.0631	wR2 = 0.1740
R indices (all data)	R1 = 0.0683	wR2 = 0.1784
Largest diff. peak and hole	7.060 and -3.420 e · Å-3	

Compound **14**



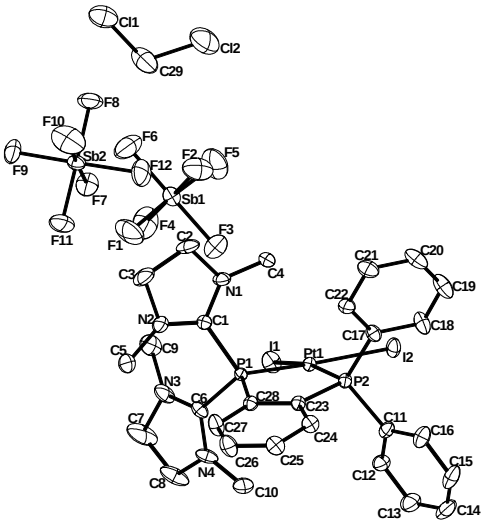
Empirical formula	$C_{62}H_{80}Cl_{14}F_{24}N_8P_4Rh_2Sb_4$	
Color	orange	
Formula weight	2706.38 $g \cdot mol^{-1}$	
Temperature	100.15 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/n$, (no. 14)**	
Unit cell dimensions	a = 13.2883(12) Å	α= 90°.
	b = 13.0485(16) Å	β= 92.308(7)°.
	c = 26.3951(12) Å	γ = 90°.
Volume	4573.0(7) $Å^3$	
Z	2	
Density (calculated)	1.965 $Mg \cdot m^{-3}$	
Absorption coefficient	2.088 mm^{-1}	
F(000)	2632 e	
Crystal size	0.10 x 0.07 x 0.04 mm^3	
θ range for data collection	2.727 to 27.500°.	
Index ranges	$-17 \leq h \leq 17$, $-16 \leq k \leq 16$, $-34 \leq l \leq 34$	
Reflections collected	87023	
Independent reflections	10476 [R_{int} = 0.0536]	
Reflections with I>2 σ (I)	9134	
Completeness to θ = 25.242°	99.6 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.94 and 0.83	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10476 / 0 / 530	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2 σ (I)]	R_1 = 0.0593	wR^2 = 0.1638
R indices (all data)	R_1 = 0.0672	wR^2 = 0.1762
Largest diff. peak and hole	3.6 and -1.8 e · $Å^{-3}$	

Compound **15**



Empirical formula	$C_{32}H_{34}ClD_6F_{12}N_6P_2RhSb_2$	
Color	orange	
Formula weight	1186.53 g · mol^{-1}	
Temperature	100.15 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 17.492(2) Å	α= 90°.
	b = 15.774(2) Å	β= 111.088(2)°.
	c = 17.985(2) Å	γ = 90°.
Volume	4629.8(11) Å^3	
Z	4	
Density (calculated)	1.702 Mg · m^{-3}	
Absorption coefficient	1.716 mm^{-1}	
F(000)	2304 e	
Crystal size	0.1 x 0.1 x 0.1 mm^3	
θ range for data collection	2.296 to 31.082°.	
Index ranges	$-25 \leq h \leq 25$, $-22 \leq k \leq 22$, $-26 \leq l \leq 26$	
Reflections collected	129694	
Independent reflections	14793 [R_{int} = 0.0730]	
Reflections with I>2 σ (I)	11201	
Completeness to θ = 25.242°	99.6 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.89 and 0.83	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14793 / 0 / 511	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2 σ (I)]	R_1 = 0.0511	wR^2 = 0.1030
R indices (all data)	R_1 = 0.0748	wR^2 = 0.1098
Largest diff. peak and hole	3.4 and -2.0 e · Å^{-3}	

Compound **17**



Empirical formula	$C_{29}\ H_{36}\ Cl_2\ F_{12}\ I_2\ N_4\ P_2\ Pt\ Sb_2$	
Color	yellow	
Formula weight	1493.85 $g{\cdot}mol^{-1}$	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	p 21/c, (no. 14)	
Unit cell dimensions	a = 17.976(6) Å	α= 90°.
	b = 14.1503(12) Å	β= 100.40(3)°.
	c = 17.202(5) Å	γ = 90°.
Volume	4303.5(19) $Å^3$	
Z	4	
Density (calculated)	2.306 $Mg{\cdot}m^{-3}$	
Absorption coefficient	6.202 mm^{-1}	
F(000)	2784 e	
Crystal size	0.16 x 0.10 x 0.01 mm^3	
θ range for data collection	2.717 to 33.132°.	
Index ranges	$-27 \leq h \leq 27$, $-21 \leq k \leq 21$, $-26 \leq l \leq 26$	
Reflections collected	135279	
Independent reflections	16334 [R_{int} = 0.0675]	
Reflections with I>2 σ (I)	14409	
Completeness to θ = 26.000°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.94105 and 0.50116	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16334 / 0 / 491	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2 σ (I)]	R_1 = 0.0342	wR^2 = 0.0832
R indices (all data)	R_1 = 0.0420	wR^2 = 0.0883
Extinction coefficient	n/a	
Largest diff. peak and hole	3.007 and -3.217 $e{\cdot}Å^{-3}$	

Computational Methods

All geometry optimizations were performed using the BP86[5] and M06L[6] functionals with BP86 being augmented by the D3 dispersion correction with BJ-damping (BP86-D3).[7] The def2-SVP[8] basis set was used for all atoms. The 28 inner-shell core electrons of the rhodium atom were described by the corresponding def2 effective core potential[9] accounting for scalar relativistic effects (def2-ecp). For the purpose of computational efficiency, the resolution-of-identity (RI) approximation[10] was applied using auxiliary basis sets to approximate Coulomb potentials in conjunction with the multipole-accelerated resolution of the identity approximation (MA-RI) method for geometry optimizations using the BP86-D3 method.[11]

Stationary points were characterized by evaluating the harmonic vibrational frequencies at the optimized geometries. Zero-point vibrational energies (ZPVE) were computed from the corresponding harmonic vibrational frequencies without scaling. Relative free energies (ΔG) were determined at standard pressure (1 bar) and at room temperature (298 K). The thermal and entropic contributions were evaluated within the rigid-rotor harmonic-oscillator approximation.[12] A quasi-harmonic approximation was applied, with all frequencies below 120 cm^{-1} being replaced by 120 cm^{-1} when computing free energies, to reduce the error arising from the harmonic-oscillator approximation for low-frequency normal modes. Solvation contributions were included for dichloromethane on the optimized gas-phase geometries employing the CPCM solvation model[13] using the same functional and the def2-TZVP basis set. Geometry optimizations at the BP86-D3 level were performed with TURBOMOLE (version-6.4)[14] and single-point CPCM solvation calculations were performed using Gaussian09.[15]

Energy decomposition and AIM analysis was performed on M06L/TZVP optimized geometries for **1** and **1-frag** using the ADF2016[16] program package at the BP86-D3 level in conjunction with a triple-ζ-quality basis set of uncontracted Slater-type orbitals (STOs)[17] augmented with two sets of polarization functions for all atoms; all electrons were included (i.e., inner core electrons were not described by a frozen core). Scalar relativistic effects were accounted for using the zeroth-order regular approximation (ZORA).[18]

Table S1. Listed are the SCF energy, zero-point vibrational energy (*ZPVE*), enthalpy correction (H_{corr}), and Gibbs free energy correction (G_{corr}) determined on the gas-phase geometries for all stationary points calculated. The single imaginary frequency (υ_i cm^{-1}) is also listed for all transition states. Single-point solvent (DCE) corrected SCF energies on the gas phase geometries are also tabulated. All energies are in atomic units.

	SCF_{gas}	SCF_{DCE}	*ZPVE*	H_{corr}	G_{corr}	υ_i (cm^{-1})
Indole	-363.610313	-363.983037	0.126566	0.133910	0.133910	
INT1	-2945.650114	-2947.924667	0.723672	0.773643	0.581752	
INT2	-2945.646471	-2947.919459	0.721767	0.773034	0.570326	
TS1	-3309.253818	-3311.883767	0.849362	0.908539	0.760442	*i*249
INT3	-3309.254503	-3311.884599	0.850505	0.909964	0.761169	
TS2	-3309.253262	-3311.878772	0.851267	0.909415	0.764536	*i*11
INT4	-3309.257990	-3311.882275	0.849743	0.908936	0.761318	
TS3	-3309.236188	-3311.863453	0.844792	0.903977	0.758172	*i*668
INT5	-3309.241225	-3311.877899	0.846696	0.906746	0.758180	
TS4	-3309.238965	-3311.875338	0.845172	0.904506	0.755677	*i*381
INT6	-3309.305895	-3311.933269	0.852409	0.911598	0.768711	
PRT	-750.469955	-751.230179	0.291830	0.309991	0.246757	
diene	-386.8205259	-387.2165137	0.161836	0.172222	0.119692	

Cartesian coordinates (Å)

Indole

C	-1.59811	-2.37151	6.51581
C	-2.54033	-2.42252	5.45702
C	-2.75010	-1.32162	4.62072
C	-2.00626	-0.13885	4.84006
C	-0.84524	-1.21721	6.76176
C	-1.05799	-0.11073	5.91958
C	-1.95275	1.15319	4.20349
C	-1.01038	1.90297	4.88645
H	-1.45556	-3.25501	7.15618
H	-3.11445	-3.34711	5.29394
H	-3.48358	-1.37146	3.80158
H	-0.11449	-1.17903	7.58385
H	-2.54091	1.48914	3.34287
H	-0.67255	2.93214	4.72031
N	-0.47460	1.14387	5.91602
H	0.23986	1.45972	6.56869

INT1

Rh	2.67081	7.16899	15.02091
Cl	1.47725	9.32244	15.19808
P	0.66205	6.22080	15.50394
P	2.88964	7.13901	17.30922
N	-1.62696	7.42921	14.20745
N	-0.90658	5.53966	13.29064
N	-0.75104	3.75647	16.30845
N	1.41973	3.50457	15.97948
C	4.56052	6.53395	14.21137
C	-0.75026	6.42162	14.29689
C	-2.47979	7.26663	13.00589
H	-2.24765	8.08861	12.29767
H	-3.54766	7.33423	13.29198
C	-2.07226	5.89134	12.45426
H	-2.86202	5.11896	12.56878
H	-1.76298	5.93620	11.39150
C	-1.72940	8.67420	14.95980
H	-0.85367	8.81160	15.61591
H	-2.68048	8.70144	15.52842
H	-1.72547	9.51205	14.23493
C	-0.09817	4.37383	12.99010
H	0.94437	4.54138	13.31878
H	-0.07965	4.23960	11.89352
H	-0.50408	3.45106	13.45551
C	0.38374	4.35000	15.89172
C	-0.48101	2.40326	16.84846
H	-1.15648	1.66374	16.37439
H	-0.68094	2.39930	17.94036
C	1.00146	2.18864	16.50591
H	1.62773	1.93760	17.38472
H	1.16949	1.41386	15.72873
C	-2.12250	4.22616	16.29032
H	-2.21115	5.15456	15.70584
H	-2.49564	4.40587	17.31906
H	-2.76127	3.45167	15.81870
C	2.77796	3.63923	15.48598
H	3.00462	4.70915	15.31355
H	2.89320	3.06527	14.54186
H	3.47621	3.23355	16.24135
C	0.10583	6.87507	17.14521
C	-1.21686	7.00899	17.60782
H	-2.06721	6.74470	16.97033
C	-1.46786	7.55069	18.87870
H	-2.50577	7.67495	19.22080
C	-0.40247	7.95358	19.70011
H	-0.60273	8.38529	20.69161
C	0.92009	7.82710	19.24538
H	1.75907	8.16663	19.87124
C	1.17931	7.29060	17.97391
C	3.49175	5.55368	18.00513

C	2.64827	4.67610	18.71572
H	1.60985	4.96602	18.93474
C	3.14436	3.44337	19.17603
H	2.49387	2.77673	19.76312
C	4.47933	3.07996	18.92875
H	4.86916	2.12155	19.30215
C	5.32635	3.95919	18.22765
H	6.37762	3.68800	18.05077
C	4.83583	5.18845	17.76544
H	5.50794	5.87725	17.23116
C	3.88254	8.41909	18.14109
C	4.54746	8.12993	19.35508
H	4.51218	7.11939	19.78716
C	5.26335	9.14271	20.01124
H	5.78270	8.91830	20.95452
C	5.32058	10.43520	19.46285
H	5.88777	11.22443	19.97819
C	4.65708	10.72012	18.25671
H	4.70094	11.73230	17.82853
C	3.93666	9.71856	17.59055
H	3.40053	9.93900	16.65504
C	4.70891	7.83997	14.79207
C	3.59115	6.37606	13.16164
H	4.67873	8.74655	14.16624
H	5.33848	7.94574	15.68829
H	5.11770	5.65823	14.58007
C	2.80934	7.48678	12.75402
H	3.38146	5.36365	12.78103
H	3.22203	8.49836	12.87985
H	-1.16615	7.57675	9.09961
C	-0.39282	7.52208	9.88044
C	0.46493	6.40847	9.94845
H	0.36403	5.59236	9.21667
C	1.48559	6.36042	10.91021
H	2.18689	5.51215	10.90550
C	1.67494	7.43008	11.81704
C	0.79939	8.54242	11.74595
H	0.94893	9.37578	12.44903
C	-0.22260	8.58604	10.78728
H	-0.86263	9.47892	10.71219

INT2

Rh	-0.03982	0.04771	-1.27125
Cl	-0.25053	-2.08276	-2.45546
P	-1.49140	-0.78327	0.12857
P	-0.12673	1.79477	0.13388
N	-3.53019	-1.46547	-1.60819
N	-2.78035	-3.27635	-0.54663
N	-1.37323	-1.73209	2.87332
N	0.50216	-1.98110	1.71014
C	1.42642	1.14074	-2.64231
C	-2.68295	-1.94232	-0.68877
C	-4.33362	-2.56877	-2.18083
H	-4.33007	-2.50152	-3.28537
H	-5.38318	-2.48760	-1.82633
C	-3.61112	-3.81868	-1.65171
H	-4.29860	-4.59761	-1.27210
H	-2.93487	-4.26766	-2.41023
C	-3.61547	-0.10687	-2.12450
H	-2.62679	0.38921	-2.00888
H	-4.39905	0.48331	-1.60833
H	-3.85355	-0.16287	-3.20300
C	-1.79173	-4.14629	0.07862
H	-0.83620	-4.10306	-0.48647
H	-2.18069	-5.17999	0.06692
H	-1.63002	-3.86292	1.13390
C	-0.80440	-1.67439	1.65213
C	-0.34584	-1.94362	3.91654
H	-0.67331	-2.72824	4.62545
H	-0.19181	-0.99669	4.47700
C	0.89079	-2.33867	3.09200
H	1.79344	-1.76391	3.37484
H	1.12934	-3.42264	3.13977
C	-2.78018	-1.64535	3.21304
H	-3.39541	-1.92225	2.33956

H	-3.06518	-0.62993	3.55657
H	-2.99392	-2.36688	4.02582
C	1.46382	-2.11097	0.62963
H	1.36424	-1.24419	-0.07139
H	1.30202	-3.03140	0.03508
H	2.47951	-2.11434	1.05846
C	-2.53253	0.57235	0.81147
C	-3.88504	0.50544	1.18875
H	-4.43352	-0.44741	1.16041
C	-4.56378	1.68046	1.55882
H	-5.62786	1.63203	1.83282
C	-3.89113	2.91342	1.56380
H	-4.42676	3.82934	1.85394
C	-2.54086	2.98823	1.17244
H	-2.02254	3.95851	1.14496
C	-1.86312	1.82433	0.77859
C	0.85962	1.49018	1.65940
C	0.33075	1.71636	2.94778
H	-0.68309	2.12495	3.06864
C	1.10637	1.43159	4.08474
H	0.69755	1.63070	5.08703
C	2.41113	0.92491	3.94488
H	3.01999	0.71831	4.83782
C	2.94028	0.69865	2.66125
H	3.96135	0.30666	2.53924
C	2.16555	0.97355	1.52483
H	2.57340	0.77644	0.52367
C	0.23316	3.49223	-0.40378
C	1.31104	4.22596	0.13312
H	1.92357	3.80229	0.94256
C	1.59473	5.50687	-0.36833
H	2.43353	6.08214	0.05019
C	0.80839	6.05442	-1.39518
H	1.03487	7.05809	-1.78392
C	-0.27008	5.32395	-1.92762
H	-0.88763	5.75685	-2.72824
C	-0.55612	4.04168	-1.44067
H	-1.40025	3.46835	-1.85532
C	0.19737	1.02812	-3.30618
C	2.37834	0.06559	-2.46631
H	-0.01792	0.16217	-3.95024
H	-0.41929	1.92681	-3.44732
H	1.70371	2.12399	-2.22250
C	3.47032	0.19303	-1.64142
H	2.14355	-0.89985	-2.94151
H	3.70103	1.20171	-1.25380
H	6.51780	-3.73561	0.42108
C	5.89688	-2.93721	-0.01157
C	4.86541	-3.25743	-0.91655
H	4.68367	-4.30742	-1.19043
C	4.07876	-2.24710	-1.47829
H	3.27268	-2.51294	-2.17826
C	4.31167	-0.88385	-1.14853
C	5.35982	-0.57835	-0.24046
H	5.56066	0.47524	0.01111
C	6.14257	-1.59366	0.32328
H	6.95841	-1.33877	1.01584

TS1

Rh	-0.90210	-0.10514	-0.13017
Cl	-2.92623	0.96768	-0.93341
P	-0.41903	-0.86756	-2.12125
P	0.93448	-1.20257	0.46634
N	-2.85064	-2.07764	-2.71301
N	-2.48693	-0.28331	-3.98612
N	1.24269	-0.50943	-4.53565
N	1.38097	1.09443	-3.01485
C	-0.84914	1.19489	2.37169
C	-1.97156	-1.13654	-3.08092
C	-4.12523	-1.89798	-3.44333
H	-4.97074	-1.92413	-2.72993
H	-4.25659	-2.72079	-4.17769
C	-3.94729	-0.52003	-4.10507
H	-4.25963	-0.50134	-5.16622
H	-4.47395	0.28223	-3.54725

C	-2.71948	-3.00171	-1.59422
H	-2.14005	-2.50456	-0.78272
H	-2.22702	-3.95011	-1.88649
H	-3.73276	-3.22344	-1.21318
C	-1.94492	1.03887	-4.28778
H	-1.77066	1.60051	-3.34482
H	-2.69199	1.58750	-4.88798
H	-1.02227	0.96642	-4.89362
C	0.74588	-0.02340	-3.38285
C	2.41543	0.27627	-4.98133
H	2.28673	0.58770	-6.03710
H	3.32833	-0.35232	-4.91789
C	2.42823	1.45690	-3.99128
H	3.39176	1.57251	-3.45691
H	2.17121	2.43119	-4.45716
C	0.74123	-1.59894	-5.34943
H	-0.28810	-1.85399	-5.04425
H	1.38675	-2.49769	-5.27349
H	0.71544	-1.27429	-6.40926
C	1.08470	2.02208	-1.93527
H	0.39772	1.54554	-1.19872
H	0.60355	2.93514	-2.34085
H	2.02626	2.30318	-1.42955
C	0.41497	-2.50889	-1.95199
C	0.37118	-3.59954	-2.83901
H	-0.20684	-3.54422	-3.77045
C	1.01860	-4.80159	-2.50229
H	0.96246	-5.66106	-3.18645
C	1.72078	-4.91098	-1.29064
H	2.22915	-5.85193	-1.03345
C	1.75083	-3.83074	-0.39072
H	2.27004	-3.92572	0.57487
C	1.08559	-2.63500	-0.70636
C	2.48577	-0.25973	0.15190
C	3.33820	-0.57096	-0.92793
H	3.15366	-1.47096	-1.53283
C	4.43709	0.25444	-1.22361
H	5.11282	-0.01209	-2.05099
C	4.69701	1.39585	-0.44621
H	5.56301	2.03489	-0.67323
C	3.85584	1.70547	0.63799
H	4.06082	2.59138	1.25719
C	2.75615	0.88707	0.92985
H	2.08996	1.14327	1.76484
C	1.12348	-1.96163	2.11935
C	2.21877	-1.70879	2.96932
H	3.04835	-1.07140	2.63179
C	2.26175	-2.29212	4.24708
H	3.12122	-2.09682	4.90542
C	1.22478	-3.13501	4.67496
H	1.26591	-3.59456	5.67302
C	0.13761	-3.40081	3.82382
H	-0.67130	-4.06871	4.15370
C	0.08066	-2.81130	2.55478
H	-0.77211	-3.01316	1.88761
C	-1.63573	0.04769	1.87202
C	-0.88632	2.37359	1.46913
H	-2.70529	0.27747	1.70558
H	-1.49255	-0.88272	2.44559
H	0.17229	0.91208	2.69443
C	0.15493	3.21550	1.23612
H	-1.83508	2.50786	0.92499
H	1.08847	3.07980	1.81063
H	0.50714	6.92680	-2.66622
C	0.42709	6.17229	-1.86964
C	-0.75241	5.41535	-1.72642
H	-1.59515	5.57786	-2.41537
C	-0.86503	4.46048	-0.70923
H	-1.77949	3.85330	-0.63484
C	0.20478	4.24611	0.19967
C	1.38368	5.01542	0.04202
H	2.22299	4.85864	0.73816
C	1.49618	5.96711	-0.98113
H	2.41788	6.55950	-1.08114
C	-0.71988	-1.30032	6.88646
C	-1.82242	-1.54600	6.03925
C	-2.20979	-0.62332	5.05303
C	-1.48097	0.56902	4.93249

C	0.02589	-0.11629	6.78331
C	-0.38513	0.79834	5.80584
C	-1.55831	1.72032	4.00211
C	-0.59188	2.65747	4.52369
H	-0.44957	-2.04067	7.65305
H	-2.39711	-2.47508	6.16480
H	-3.07856	-0.81946	4.40976
H	0.87407	0.08675	7.45247
H	-2.52769	2.10366	3.64877
H	-0.35761	3.66523	4.15955
N	0.11748	2.08098	5.50561
H	0.90819	2.51890	5.98696

INT3

Rh	-0.85982	0.15598	-0.24117
Cl	-2.58691	1.71699	-0.92085
P	-0.20748	-0.21172	-2.30028
P	0.62637	-1.41619	0.25705
N	-2.69782	-0.71348	-3.45489
N	-1.84224	1.24738	-4.08373
N	1.72740	0.34470	-4.47860
N	2.09559	1.37542	-2.55459
C	-1.00332	0.84943	2.56392
C	-1.62247	0.08407	-3.44379
C	-3.80991	-0.06446	-4.18451
H	-4.72194	-0.07835	-3.55730
H	-4.01850	-0.61855	-5.12368
C	-3.28040	1.36210	-4.42872
H	-3.40395	1.69838	-5.47588
H	-3.74292	2.10205	-3.74370
C	-2.89509	-1.90816	-2.64393
H	-2.38621	-1.76617	-1.66352
H	-2.51421	-2.82207	-3.14058
H	-3.97877	-2.02275	-2.46154
C	-1.02672	2.44778	-3.92648
H	-0.77075	2.59681	-2.85602
H	-1.62628	3.31608	-4.25199
H	-0.11860	2.41109	-4.55909
C	1.25647	0.59561	-3.24340
C	3.06995	0.93935	-4.66921
H	3.07023	1.59396	-5.56434
H	3.81357	0.13276	-4.83618
C	3.29546	1.70478	-3.35000
H	4.19603	1.37340	-2.79513
H	3.35774	2.80494	-3.47983
C	1.07530	-0.32634	-5.58549
H	0.00410	-0.46907	-5.36449
H	1.54671	-1.30710	-5.80002
H	1.15895	0.30658	-6.49252
C	1.90302	2.04554	-1.27749
H	1.01333	1.62769	-0.75707
H	1.75058	3.12993	-1.45062
H	2.80028	1.90022	-0.64854
C	0.29590	-1.98507	-2.46297
C	0.23662	-2.80058	-3.60752
H	-0.15474	-2.41111	-4.55541
C	0.62128	-4.15045	-3.52626
H	0.55035	-4.79212	-4.41690
C	1.08061	-4.68251	-2.31006
H	1.38491	-5.73799	-2.25195
C	1.12820	-3.87596	-1.15944
H	1.45955	-4.29780	-0.19867
C	0.72179	-2.53287	-1.22467
C	2.36035	-0.81209	0.41008
C	3.32281	-1.05518	-0.59200
H	3.08724	-1.72663	-1.43074
C	4.59111	-0.45363	-0.51709
H	5.34326	-0.66773	-1.29201
C	4.91350	0.39167	0.55798
H	5.90948	0.85443	0.61900
C	3.96155	0.62877	1.56621
H	4.21154	1.28164	2.41574
C	2.69338	0.03718	1.48772
H	1.94378	0.24459	2.26425
C	0.36976	-2.58323	1.64620

C	1.28834	-2.75580	2.69975
H	2.24609	-2.21634	2.69557
C	0.99186	-3.64146	3.75036
H	1.71507	-3.77620	4.56825
C	-0.20884	-4.36704	3.74643
H	-0.43042	-5.06837	4.56419
C	-1.12428	-4.20473	2.69122
H	-2.06267	-4.77882	2.68017
C	-0.84378	-3.30886	1.65177
H	-1.56331	-3.17238	0.82883
C	-1.81027	-0.03374	1.64815
C	-0.71456	2.16226	1.89763
H	-2.82468	0.37158	1.46363
H	-1.85986	-1.08142	1.99064
H	-0.06537	0.34428	2.87724
C	0.49254	2.78219	1.88553
H	-1.56112	2.59108	1.33712
H	1.32088	2.34895	2.47384
H	1.98910	6.88451	-1.28805
C	1.67509	6.05501	-0.63710
C	0.37698	5.51837	-0.74767
H	-0.32371	5.92795	-1.49124
C	-0.03281	4.46885	0.08324
H	-1.03286	4.02952	-0.05009
C	0.85228	3.93425	1.05591
C	2.15314	4.48383	1.15552
H	2.85328	4.07340	1.90054
C	2.56240	5.53243	0.31904
H	3.57564	5.94981	0.41767
C	-1.62118	-2.35895	6.53281
C	-2.52528	-2.43332	5.45266
C	-2.69932	-1.35880	4.56148
C	-1.95424	-0.19289	4.77310
C	-0.86783	-1.19773	6.76802
C	-1.06568	-0.13882	5.87517
C	-1.82206	1.09273	4.01126
C	-0.94799	1.89619	4.87513
H	-1.51357	-3.21678	7.21192
H	-3.11398	-3.35070	5.30999
H	-3.41598	-1.42856	3.73250
H	-0.17464	-1.12537	7.61812
H	-2.75435	1.60300	3.70309
H	-0.60952	2.92780	4.71454
N	-0.48735	1.15325	5.87688
H	0.19553	1.47491	6.57173

TS2

Rh	-0.56583	-0.25211	0.15798
Cl	-2.91348	0.31350	0.56944
P	-0.67917	-0.32085	-2.04991
P	1.34250	-1.36157	-0.07999
N	-2.92313	-2.01561	-2.27748
N	-3.40827	0.14619	-2.48186
N	-0.96155	1.17679	-4.59208
N	0.57782	1.90230	-3.17501
C	-0.17082	0.88278	2.82622
C	-2.43095	-0.77356	-2.43014
C	-4.37742	-1.95096	-1.99733
H	-4.54206	-2.18554	-0.92521
H	-4.92268	-2.68664	-2.61926
C	-4.73325	-0.49014	-2.32928
H	-5.31458	-0.38684	-3.26985
H	-5.28366	0.00871	-1.50871
C	-2.15395	-3.18972	-1.87952
H	-1.58728	-2.97454	-0.94681
H	-1.44639	-3.49621	-2.67086
H	-2.85851	-4.02012	-1.69930
C	-3.26250	1.58856	-2.42889
H	-2.27655	1.85651	-2.00675
H	-4.02496	1.99230	-1.73793
H	-3.39230	2.05859	-3.42653
C	-0.35593	0.97449	-3.40465
C	-0.47973	2.43332	-5.21360
H	-1.29717	3.18551	-5.20728
H	-0.19031	2.24928	-6.26685

C	0.70559	2.83039	-4.31447
H	1.69364	2.68574	-4.80042
H	0.64656	3.87147	-3.93979
C	-1.92869	0.35891	-5.29972
H	-2.07325	-0.60622	-4.78763
H	-1.55962	0.16218	-6.32711
H	-2.90967	0.87269	-5.37909
C	1.53490	1.94877	-2.08164
H	1.09364	1.47975	-1.17884
H	1.76962	3.00424	-1.86050
H	2.46502	1.40847	-2.35179
C	0.44422	-1.61992	-2.72382
C	0.44157	-2.11377	-4.04289
H	-0.24619	-1.70630	-4.79653
C	1.30541	-3.16311	-4.39531
H	1.29246	-3.56272	-5.41995
C	2.17400	-3.71234	-3.43498
H	2.83790	-4.54564	-3.70866
C	2.20041	-3.19891	-2.12760
H	2.88230	-3.62831	-1.37802
C	1.34703	-2.13975	-1.76728
C	2.93147	-0.43144	-0.04980
C	3.87492	-0.45160	-1.09740
H	3.70981	-1.08349	-1.98180
C	5.03506	0.33852	-1.01840
H	5.76741	0.31455	-1.83921
C	5.26547	1.14710	0.10599
H	6.17646	1.76053	0.16700
C	4.33262	1.16179	1.15856
H	4.51594	1.78369	2.04768
C	3.17019	0.38314	1.07784
H	2.43684	0.39928	1.89640
C	1.65612	-2.80947	1.00271
C	2.95184	-3.16475	1.42752
H	3.81377	-2.53606	1.15894
C	3.14007	-4.32371	2.19992
H	4.15221	-4.59917	2.53154
C	2.04220	-5.12737	2.54744
H	2.19458	-6.03464	3.15067
C	0.74697	-4.76915	2.13092
H	-0.11438	-5.39405	2.41060
C	0.55251	-3.61102	1.36610
H	-0.45984	-3.30133	1.05953
C	-0.41192	-0.52406	2.25687
C	-0.37671	1.96729	1.79820
H	-1.42177	-0.91337	2.48466
H	0.34602	-1.24199	2.61601
H	0.86177	0.95584	3.22933
C	0.56670	2.85237	1.37925
H	-1.40681	2.03889	1.41415
H	1.58277	2.81120	1.80881
H	-0.04357	6.34160	-2.70490
C	0.07630	5.62875	-1.87516
C	-0.93698	4.69274	-1.58634
H	-1.85212	4.67085	-2.19904
C	-0.79695	3.80144	-0.51632
H	-1.58600	3.06338	-0.30808
C	0.36342	3.82430	0.30114
C	1.37011	4.77414	0.00253
H	2.28026	4.80386	0.62179
C	1.23016	5.66568	-1.07184
H	2.02235	6.40025	-1.28001
C	-0.26121	-0.77828	7.78700
C	-0.64895	-1.62579	6.72830
C	-0.98545	-1.11682	5.45895
C	-0.92752	0.26725	5.26114
C	-0.19701	0.61359	7.61193
C	-0.53612	1.09311	6.34251
C	-1.16807	1.14886	4.06020
C	-0.95361	2.50720	4.61352
H	-0.00958	-1.21064	8.76597
H	-0.69350	-2.71088	6.90123
H	-1.29019	-1.79152	4.64861
H	0.09782	1.28301	8.43257
H	-2.18191	1.05232	3.60796
H	-1.02625	3.46575	4.08347
N	-0.57049	2.43189	5.87756
H	-0.32255	3.24266	6.45745

INT4

Rh	-0.53323	-0.02589	-0.46127
Cl	-1.06995	1.83812	-1.95075
P	1.17394	-0.88887	-1.55036
P	-0.46830	-1.92054	0.65622
N	0.62515	-0.65245	-4.24621
N	2.80013	-0.33350	-3.95049
N	3.53423	-0.87763	0.15639
N	3.00431	1.06453	-0.77270
C	-1.87938	2.06966	1.41311
C	1.63802	-0.69301	-3.36709
C	1.10924	-0.31538	-5.59920
H	0.48530	0.49037	-6.03201
H	1.03075	-1.20642	-6.25871
C	2.56574	0.12114	-5.34118
H	3.29221	-0.35640	-6.02701
H	2.70198	1.22186	-5.40516
C	-0.74745	-1.07074	-4.01086
H	-1.00058	-0.90429	-2.93897
H	-0.88101	-2.14350	-4.26387
H	-1.42444	-0.45491	-4.63025
C	4.14390	-0.43102	-3.41248
H	4.55346	0.56259	-3.13263
H	4.81115	-0.87420	-4.17856
H	4.15218	-1.08979	-2.52687
C	2.72253	-0.25000	-0.71578
C	4.37102	0.10403	0.88196
H	5.42650	-0.23121	0.88869
H	4.01747	0.16581	1.93258
C	4.14229	1.40652	0.10153
H	3.87627	2.26106	0.75198
H	5.01472	1.70446	-0.51955
C	3.60879	-2.27262	0.55764
H	2.92943	-2.89075	-0.04587
H	3.33332	-2.37326	1.62640
H	4.64755	-2.63660	0.42186
C	2.38226	2.06997	-1.61122
H	2.95382	2.22620	-2.55166
H	2.36461	3.02250	-1.04992
H	1.32954	1.80247	-1.84101
C	1.15037	-2.72371	-1.44433
C	1.79861	-3.61007	-2.32514
H	2.46845	-3.22955	-3.11145
C	1.58218	-4.99322	-2.19782
H	2.07635	-5.69107	-2.88966
C	0.72840	-5.48480	-1.19477
H	0.55429	-6.56738	-1.10682
C	0.08400	-4.60008	-0.31049
H	-0.60434	-4.98816	0.45544
C	0.29005	-3.21645	-0.43135
C	0.60509	-1.96054	2.15132
C	0.86199	-3.15359	2.85972
H	0.37409	-4.09344	2.56168
C	1.74596	-3.14837	3.95001
H	1.94440	-4.08084	4.49891
C	2.37184	-1.95163	4.34386
H	3.05845	-1.94868	5.20343
C	2.11076	-0.76009	3.64496
H	2.58632	0.17993	3.96233
C	1.23522	-0.76160	2.54674
H	1.02829	0.16190	1.97997
C	-2.07640	-2.62622	1.15182
C	-2.48033	-2.71172	2.49819
H	-1.78366	-2.43936	3.30442
C	-3.78079	-3.14407	2.81022
H	-4.09416	-3.21239	3.86242
C	-4.67576	-3.48913	1.78549
H	-5.69095	-3.83168	2.03474
C	-4.27507	-3.39824	0.43921
H	-4.97517	-3.67234	-0.36413
C	-2.98341	-2.95910	0.12051
H	-2.67254	-2.86623	-0.93230
C	-1.75343	0.55469	1.19609
C	-0.52417	2.73137	1.32636

H	-2.74919	0.07832	1.11481
H	-1.30709	0.15569	2.12993
H	-2.29825	2.22792	2.43330
C	0.32770	2.88048	2.36702
H	-0.20035	3.00793	0.30828
H	0.01761	2.52676	3.36708
H	5.35436	4.87489	2.10118
C	4.33593	4.46139	2.14233
C	3.38228	4.82677	1.17339
H	3.65440	5.53517	0.37620
C	2.07808	4.31574	1.23512
H	1.32949	4.64434	0.49828
C	1.68897	3.43114	2.27296
C	2.65389	3.09551	3.25345
H	2.35748	2.44969	4.09492
C	3.96450	3.59422	3.18458
H	4.69375	3.32602	3.96378
C	-6.93496	1.73923	-0.52055
C	-5.99506	0.69225	-0.64142
C	-4.63115	0.88466	-0.36021
C	-4.21456	2.14924	0.08284
C	-6.53555	3.02417	-0.12514
C	-5.17545	3.18819	0.16439
C	-2.86942	2.74088	0.40277
C	-3.18758	4.14114	0.69649
H	-7.99290	1.55097	-0.75302
H	-6.33920	-0.29881	-0.97104
H	-3.91202	0.06610	-0.49489
H	-7.25332	3.85393	-0.05602
H	-2.27184	2.71372	-0.59022
H	-2.49849	4.93457	1.01597
N	-4.48485	4.36323	0.54469
H	-4.93766	5.27614	0.67046

TS3

Rh	-0.35559	0.19339	-0.44760
Cl	-0.10737	1.51940	-2.42541
P	1.26441	-1.34127	-1.05218
P	-1.08820	-1.47335	0.83965
N	1.24487	-1.34721	-3.79093
N	3.34242	-1.16574	-3.06608
N	3.16037	-1.97193	1.03407
N	3.30789	0.06804	0.16162
C	-0.70268	2.76742	0.97903
C	2.05645	-1.41729	-2.71728
C	2.01419	-1.08786	-5.02173
H	1.54788	-0.25301	-5.57964
H	2.00983	-1.98909	-5.67231
C	3.41303	-0.73207	-4.48089
H	4.22874	-1.26856	-5.00297
H	3.62403	0.35693	-4.53086
C	-0.18510	-1.59230	-3.82485
H	-0.65423	-1.22080	-2.89147
H	-0.40615	-2.67404	-3.94332
H	-0.62607	-1.02595	-4.66450
C	4.54809	-1.49653	-2.32875
H	5.06134	-0.59509	-1.93365
H	5.25445	-2.02150	-3.00337
H	4.30761	-2.17747	-1.49328
C	2.71704	-1.13904	0.07796
C	4.10671	-1.27523	1.93228
H	5.03354	-1.87243	2.03957
H	3.64137	-1.17850	2.93515
C	4.32876	0.07723	1.22750
H	4.16909	0.95091	1.88972
H	5.34039	0.17407	0.77834
C	2.78894	-3.34747	1.31890
H	2.02548	-3.69487	0.60626
H	2.37560	-3.41628	2.34459
H	3.68329	-3.99975	1.24810
C	3.11877	1.23155	-0.69193
H	3.95649	1.33723	-1.41270
H	3.08261	2.14562	-0.06920
H	2.15863	1.16776	-1.24299
C	0.45339	-2.97672	-0.93725

C	0.82118	-4.10425	-1.69958
H	1.76898	-4.11188	-2.25931
C	-0.03798	-5.21430	-1.75610
H	0.24250	-6.09233	-2.35620
C	-1.26092	-5.19737	-1.06231
H	-1.93942	-6.06079	-1.12709
C	-1.62501	-4.08057	-0.28794
H	-2.58728	-4.06358	0.24658
C	-0.76899	-2.97058	-0.21098
C	-0.24631	-2.03985	2.39086
C	-0.49823	-3.34379	2.87842
H	-1.18273	-4.01544	2.34127
C	0.12727	-3.80324	4.04730
H	-0.08452	-4.81789	4.41570
C	1.01626	-2.96870	4.74699
H	1.49512	-3.32332	5.67163
C	1.28567	-1.67909	4.25960
H	1.96949	-1.01569	4.81123
C	0.66696	-1.21965	3.08416
H	0.89267	-0.21439	2.71259
C	-2.87828	-1.50579	1.18949
C	-3.42684	-1.96824	2.40245
H	-2.77424	-2.28843	3.22625
C	-4.82105	-2.00848	2.56406
H	-5.24844	-2.37013	3.51082
C	-5.66512	-1.58324	1.52674
H	-6.75650	-1.61564	1.65888
C	-5.11864	-1.09962	0.32481
H	-5.78008	-0.74701	-0.47937
C	-3.73018	-1.05256	0.15623
H	-3.29467	-0.65523	-0.77460
C	-0.15568	1.35820	1.29526
C	0.27873	3.54777	0.14591
H	-0.71240	0.92642	2.14878
H	0.92755	1.38444	1.53820
H	-0.83225	3.29447	1.95456
C	1.32469	4.22785	0.67000
H	0.20753	3.42135	-0.94390
H	1.38604	4.34794	1.76776
H	5.51625	6.32798	-2.02346
C	4.66152	5.89701	-1.48141
C	3.69947	5.13227	-2.16852
H	3.80288	4.96745	-3.25194
C	2.60576	4.58865	-1.48482
H	1.86703	3.98644	-2.03622
C	2.44308	4.80339	-0.09113
C	3.42227	5.56985	0.58496
H	3.30953	5.75093	1.66561
C	4.51866	6.11256	-0.10142
H	5.26160	6.71455	0.44264
C	-5.94937	1.81750	1.95130
C	-4.85946	1.43448	2.76606
C	-3.53493	1.62572	2.34878
C	-3.30207	2.23117	1.10158
C	-5.74588	2.41130	0.69836
C	-4.41636	2.61400	0.30131
C	-2.08043	2.57769	0.34502
C	-2.55438	3.27595	-0.81069
H	-6.97614	1.65548	2.30969
H	-5.05679	0.98065	3.74742
H	-2.70092	1.32333	2.99787
H	-6.59196	2.72099	0.06818
H	-1.72595	1.29031	-0.19383
H	-1.97456	3.73103	-1.61978
N	-3.90634	3.23017	-0.84807
H	-4.47786	3.60791	-1.60691

INT5

Rh	-0.15266	0.33650	-0.59145
Cl	1.35463	1.30217	-2.13342
P	0.86490	-1.76159	-0.52035
P	-1.91391	-0.80470	0.23144
N	1.84565	-1.93221	-3.08044
N	3.39181	-2.65325	-1.65465
N	1.44546	-2.85659	2.08755

N	2.70903	-1.14750	1.43009
C	0.26391	2.95648	0.92174
C	2.11227	-2.25238	-1.80651
C	3.02878	-2.13996	-3.93898
H	3.23412	-1.21201	-4.50715
H	2.82903	-2.95715	-4.66422
C	4.13958	-2.47796	-2.92354
H	4.68698	-3.40869	-3.17006
H	4.88007	-1.65919	-2.80985
C	0.56322	-1.57601	-3.66507
H	-0.08996	-1.10371	-2.90749
H	0.06058	-2.47739	-4.07466
H	0.72500	-0.83356	-4.46713
C	3.99610	-3.35228	-0.53388
H	4.68096	-2.69930	0.04564
H	4.58623	-4.20678	-0.92117
H	3.21488	-3.75463	0.13408
C	1.76513	-2.03779	1.07396
C	2.16437	-2.45464	3.31829
H	2.63710	-3.33908	3.78769
H	1.42821	-2.03343	4.03480
C	3.18021	-1.41629	2.80435
H	3.18557	-0.47563	3.38860
H	4.22150	-1.80317	2.77341
C	0.46871	-3.93154	2.14473
H	-0.04626	-4.03511	1.17724
H	-0.28429	-3.70787	2.92574
H	0.97571	-4.88495	2.39749
C	3.35135	-0.13502	0.60379
H	4.32453	-0.49622	0.21032
H	3.54147	0.76882	1.21130
H	2.69531	0.16850	-0.23844
C	-0.48238	-2.95486	-0.85315
C	-0.29900	-4.20786	-1.47156
H	0.71169	-4.62654	-1.59714
C	-1.41518	-4.91523	-1.94812
H	-1.27725	-5.89145	-2.43552
C	-2.70382	-4.36577	-1.82324
H	-3.57206	-4.91210	-2.22060
C	-2.89152	-3.11964	-1.19766
H	-3.89956	-2.68584	-1.10781
C	-1.78724	-2.41150	-0.69687
C	-1.99616	-1.50225	1.94764
C	-2.84587	-2.60504	2.20210
H	-3.43291	-3.05437	1.38882
C	-2.94805	-3.14710	3.49228
H	-3.62156	-3.99779	3.67340
C	-2.19731	-2.60262	4.54877
H	-2.28793	-3.01860	5.56304
C	-1.33528	-1.52155	4.30076
H	-0.75540	-1.08033	5.12590
C	-1.22971	-0.97735	3.00893
H	-0.55494	-0.13231	2.83652
C	-3.56983	-0.14351	-0.14100
C	-4.68633	-0.35489	0.69367
H	-4.57979	-0.87894	1.65314
C	-5.94533	0.12931	0.30481
H	-6.81508	-0.03276	0.95820
C	-6.09125	0.82779	-0.90341
H	-7.07881	1.20989	-1.20069
C	-4.97324	1.06176	-1.72288
H	-5.08109	1.63490	-2.65446
C	-3.71383	0.58337	-1.34449
H	-2.83193	0.79041	-1.97056
C	-0.04061	1.46399	1.17040
C	1.70012	3.17118	0.53403
H	-0.99725	1.38209	1.71476
H	0.77294	0.98145	1.75464
H	0.12644	3.39535	1.94415
C	2.70520	3.27926	1.43402
H	1.92772	3.11169	-0.54052
H	2.44775	3.35476	2.50722
H	8.02070	3.15237	0.45196
C	6.93800	3.17605	0.64517
C	6.02582	2.95468	-0.40452
H	6.39857	2.75899	-1.42161
C	4.64712	2.99390	-0.16616
H	3.94709	2.80889	-0.99534

C	4.14390	3.26399	1.13327
C	5.07487	3.47785	2.17827
H	4.70224	3.69617	3.19172
C	6.45642	3.43675	1.93805
H	7.16126	3.61981	2.76275
C	-4.98091	3.96135	-0.08668
C	-4.45469	3.25830	1.02417
C	-3.07837	3.05630	1.16795
C	-2.20023	3.56836	0.18468
C	-4.14211	4.48176	-1.07904
C	-2.75945	4.27978	-0.92918
C	-0.75609	3.58497	0.01136
C	-0.50788	4.30233	-1.15817
H	-6.06731	4.11233	-0.16529
H	-5.14238	2.87424	1.79108
H	-2.69353	2.52949	2.05412
H	-4.54991	5.04280	-1.93261
H	-1.08719	1.59656	-0.77598
H	0.44529	4.54955	-1.63535
N	-1.70067	4.70217	-1.71752
H	-1.78747	5.26147	-2.56566

TS4

Rh	-0.06294	0.34703	-0.19260
Cl	1.00395	2.01412	-1.55453
P	1.47993	-1.25676	-0.76365
P	-1.22498	-1.43807	0.49323
N	1.82508	-0.63884	-3.40933
N	3.81267	-1.02628	-2.48739
N	2.87883	-2.48241	1.44706
N	3.48590	-0.39714	0.95943
C	-1.41712	2.90446	1.00877
C	2.47784	-1.04045	-2.31486
C	2.77058	-0.23625	-4.47024
H	2.59101	0.82929	-4.71640
H	2.60003	-0.84230	-5.38318
C	4.15261	-0.47369	-3.82173
H	4.77543	-1.20395	-4.37682
H	4.73794	0.46037	-3.70274
C	0.38723	-0.57918	-3.61749
H	-0.12744	-0.36984	-2.65239
H	0.01640	-1.53249	-4.04758
H	0.16036	0.25775	-4.30179
C	4.83798	-1.66021	-1.67599
H	5.44716	-0.91549	-1.12423
H	5.51579	-2.23359	-2.33970
H	4.38222	-2.36867	-0.96252
C	2.74262	-1.45416	0.58820
C	3.71358	-2.07671	2.60100
H	4.49357	-2.83984	2.78975
H	3.06394	-2.01451	3.49955
C	4.27932	-0.71479	2.16334
H	4.14546	0.08857	2.91441
H	5.35741	-0.75292	1.89711
C	2.20808	-3.77192	1.50066
H	1.62061	-3.94625	0.58780
H	1.52972	-3.80628	2.37707
H	2.96653	-4.57341	1.60317
C	3.64111	0.89705	0.31404
H	4.62699	0.96662	-0.19118
H	3.59483	1.68974	1.08670
H	2.82402	1.10105	-0.40823
C	0.59272	-2.81368	-1.11777
C	1.07325	-3.84479	-1.94843
H	2.10102	-3.81660	-2.34267
C	0.22167	-4.91091	-2.28214
H	0.58397	-5.71697	-2.93677
C	-1.09809	-4.93883	-1.79517
H	-1.76531	-5.76762	-2.07465
C	-1.57750	-3.90838	-0.96584
H	-2.61889	-3.91962	-0.60931
C	-0.73431	-2.84058	-0.61816
C	-0.80883	-2.13452	2.14389
C	-1.29447	-3.39376	2.56104
H	-1.95809	-3.97920	1.90760

C	-0.92926	-3.90944	3.81419
H	-1.31488	-4.88805	4.13613
C	-0.08046	-3.17319	4.66095
H	0.19048	-3.57300	5.64935
C	0.41245	-1.92363	4.24642
H	1.05798	-1.33716	4.91812
C	0.05829	-1.40947	2.98779
H	0.44955	-0.43752	2.65046
C	-3.03570	-1.32953	0.36879
C	-3.89877	-1.62643	1.44261
H	-3.49612	-1.96109	2.40916
C	-5.28573	-1.47814	1.27707
H	-5.96024	-1.70712	2.11498
C	-5.80711	-1.02708	0.05504
H	-6.89252	-0.90279	-0.06660
C	-4.94483	-0.71345	-1.01058
H	-5.35418	-0.32916	-1.95516
C	-3.56227	-0.85564	-0.85565
H	-2.88323	-0.58200	-1.67790
C	-1.25237	1.40023	1.26916
C	-0.07265	3.59177	0.90675
H	-2.23575	0.92678	1.45201
H	-0.58470	1.19323	2.12977
H	-1.93530	3.29073	1.92314
C	0.90817	3.39049	1.81766
H	0.11227	4.22222	0.02561
H	0.66654	2.79369	2.71669
H	6.17453	4.55123	1.48713
C	5.09906	4.32916	1.55243
C	4.25036	4.60398	0.46286
H	4.66666	5.03700	-0.45938
C	2.87815	4.33572	0.54221
H	2.23572	4.52599	-0.32860
C	2.31462	3.78666	1.72141
C	3.18183	3.51929	2.81153
H	2.75717	3.10777	3.74167
C	4.55736	3.78801	2.73077
H	5.20724	3.59100	3.59698
C	-6.50135	2.39980	-0.70833
C	-6.01146	2.17455	0.60186
C	-4.65791	2.34867	0.90899
C	-3.77440	2.76497	-0.11189
C	-5.64989	2.80856	-1.74356
C	-4.29226	2.99021	-1.42916
C	-2.36001	3.08474	-0.14941
C	-2.07982	3.48037	-1.45811
H	-7.57333	2.26585	-0.91534
H	-6.71222	1.86839	1.39203
H	-4.29776	2.18388	1.93563
H	-6.03717	3.00121	-2.75492
H	-1.43165	1.10060	-0.49818
H	-1.12624	3.77672	-1.90604
N	-3.23068	3.41593	-2.21549
H	-3.30303	3.70600	-3.18994

INT6

Rh	-0.87954	-0.26222	-0.00152
Cl	-3.12288	-1.09254	0.32340
P	-0.93818	-1.03983	-2.05208
P	1.31147	0.08657	-0.38832
N	-1.25118	-3.79515	-1.74027
N	-3.15543	-2.83070	-2.36648
N	-2.11648	-0.47655	-4.68219
N	-1.96947	1.26540	-3.31890
C	-0.26179	-0.61801	3.20463
C	-1.84014	-2.65994	-2.14883
C	-2.22512	-4.90829	-1.73506
H	-2.15935	-5.46426	-0.78011
H	-1.99427	-5.61107	-2.56433
C	-3.56806	-4.18019	-1.91476
H	-4.22942	-4.65863	-2.66192
H	-4.12378	-4.06575	-0.95966
C	0.12936	-3.97848	-1.31924
H	0.49101	-3.06540	-0.81035
H	0.80005	-4.21336	-2.17037

H	0.16270	-4.81264	-0.59458
C	-4.17033	-1.81655	-2.61481
H	-3.83087	-0.83046	-2.25270
H	-5.06588	-2.06844	-2.01683
H	-4.45874	-1.78561	-3.68543
C	-1.76717	-0.05050	-3.45231
C	-2.64250	0.64008	-5.50166
H	-3.69510	0.42777	-5.78213
H	-2.05171	0.72808	-6.43578
C	-2.49474	1.85501	-4.56978
H	-1.77691	2.61328	-4.94382
H	-3.45291	2.37007	-4.35786
C	-2.07975	-1.79517	-5.28554
H	-1.79023	-2.56123	-4.55049
H	-1.36502	-1.80964	-6.13400
H	-3.08412	-2.05179	-5.68097
C	-1.72860	2.14517	-2.18573
H	-1.32256	1.55662	-1.33383
H	-2.67608	2.62190	-1.86664
H	-1.00236	2.93038	-2.46990
C	0.72478	-1.25620	-2.80666
C	1.03800	-1.92749	-4.00690
H	0.26462	-2.44681	-4.58416
C	2.36529	-1.96286	-4.45772
H	2.61263	-2.49761	-5.38650
C	3.37828	-1.31831	-3.72404
H	4.41695	-1.33955	-4.08522
C	3.07064	-0.66475	-2.52195
H	3.86933	-0.18418	-1.93870
C	1.74563	-0.63790	-2.04854
C	1.94957	1.79775	-0.52229
C	1.79839	2.48930	-1.74350
H	1.40998	1.96169	-2.62855
C	2.16010	3.84119	-1.83968
H	2.05114	4.37160	-2.79741
C	2.67691	4.51460	-0.71872
H	2.96572	5.57297	-0.79698
C	2.82985	3.83075	0.49889
H	3.23024	4.34908	1.38244
C	2.46432	2.47937	0.60268
H	2.57707	1.97168	1.57177
C	2.48829	-0.81955	0.68848
C	3.82816	-0.41386	0.87051
H	4.20185	0.50903	0.40445
C	4.68702	-1.18062	1.67321
H	5.72633	-0.85384	1.82407
C	4.22152	-2.35447	2.29022
H	4.89626	-2.94406	2.92802
C	2.89361	-2.77109	2.09723
H	2.52485	-3.68545	2.58477
C	2.03003	-2.00657	1.29973
H	0.97742	-2.30338	1.16981
C	-0.87624	-1.99292	3.47775
C	-1.11608	0.21467	2.26701
H	-1.88106	-1.90128	3.93701
H	-0.23864	-2.57898	4.16690
H	0.73714	-0.75545	2.75159
C	-0.66733	1.36394	1.61070
H	-2.20193	0.07941	2.39423
H	0.39253	1.63375	1.73723
H	-3.67858	5.47960	-0.19049
C	-3.07351	4.63169	0.16374
C	-3.70099	3.46216	0.63529
H	-4.79914	3.39448	0.64876
C	-2.93698	2.38656	1.10434
H	-3.44288	1.47389	1.44834
C	-1.52152	2.45949	1.11275
C	-0.90276	3.64161	0.63837
H	0.19264	3.71732	0.65092
C	-1.67032	4.71576	0.16775
H	-1.17009	5.63100	-0.18233
C	3.11474	2.77474	5.64173
C	3.37419	1.97124	4.50236
C	2.40402	1.09412	4.00381
C	1.14896	1.02600	4.64962
C	1.88858	2.70984	6.31727
C	0.91412	1.83222	5.81080
C	-0.04468	0.24691	4.42133

C	-0.94710	0.59903	5.42406
H	3.89754	3.45096	6.01520
H	4.36133	2.02664	4.01909
H	2.62655	0.43994	3.14769
H	1.70303	3.32070	7.21274
H	-1.00559	-2.55795	2.53142
H	-1.96811	0.24757	5.61090
N	-0.36779	1.54118	6.25143
H	-0.80550	1.93546	7.08377

PRT

C	-1.82886	3.22510	-0.36010
C	-2.87203	2.12737	-0.08543
C	-0.73015	3.32350	0.67114
H	-3.65231	2.13540	-0.87095
H	-3.36505	2.27088	0.89764
H	-2.36260	4.20549	-0.34840
C	-0.51246	2.46720	1.69583
H	-0.04065	4.17241	0.51861
H	-1.20709	1.62114	1.83190
H	3.41449	2.59422	5.42068
C	2.62068	2.57519	4.65884
C	2.60512	3.53137	3.62646
H	3.39056	4.30124	3.57904
C	1.59719	3.51135	2.65555
H	1.60522	4.26627	1.85534
C	0.57173	2.53375	2.68829
C	0.60587	1.57809	3.73225
H	-0.18160	0.80876	3.77426
C	1.61484	1.59687	4.70613
H	1.61533	0.84226	5.50759
C	-2.45376	3.98429	-5.69982
C	-3.34958	4.37745	-4.67353
C	-3.05787	4.13372	-3.32710
C	-1.84786	3.48414	-2.99303
C	-1.24628	3.34001	-5.40284
C	-0.95534	3.09533	-4.04874
C	-1.23482	3.08298	-1.74583
C	-0.02864	2.48112	-2.07691
H	-2.71114	4.18912	-6.74995
H	-4.28899	4.88245	-4.94451
H	-3.76036	4.44458	-2.53853
H	-0.55245	3.03649	-6.20144
H	-2.40018	1.12425	-0.09962
H	0.72916	2.04210	-1.41820
N	0.13691	2.48927	-3.45429
H	0.94618	2.12124	-3.94986

diene

C	-1.29541	0.55016	1.88530
C	-2.47475	0.03245	1.46116
C	-0.79713	1.86395	1.53076
H	-3.14446	0.60486	0.79845
H	-2.80434	-0.97306	1.76160
H	-0.65139	-0.05496	2.54929
C	0.39415	2.36506	1.96724
H	-1.43891	2.47073	0.86778
H	1.00484	1.72307	2.62739
H	2.65938	7.15810	0.91654
C	2.19096	6.18461	1.12575
C	0.93301	5.87098	0.57759
H	0.41531	6.60176	-0.06242
C	0.33328	4.63488	0.84022
H	-0.65053	4.40980	0.40252
C	0.97530	3.67230	1.66151
C	2.24103	4.00704	2.20508
H	2.75535	3.27318	2.84561
C	2.84217	5.24514	1.94157
H	3.82615	5.47894	2.37585

1

C	1.43288	3.98319	5.20411
C	0.22531	2.88019	6.85053
H	0.15961	1.79753	7.01134
H	-0.70537	3.35262	7.20022
C	1.48738	3.49657	7.47298
H	1.27832	4.14909	8.32931
H	2.21983	2.73309	7.77210
C	-0.60593	2.70935	4.46475
H	-0.51165	3.24136	3.51674
H	-1.60533	2.88897	4.88552
H	-0.49393	1.63197	4.28078
C	3.31867	4.97266	6.51158
H	4.11229	4.24160	6.72750
H	3.24700	5.68439	7.34376
H	3.56849	5.51051	5.59121
C	0.80034	5.68559	2.90824
C	0.00001	7.21987	1.33933
H	-0.57374	6.95452	0.44202
H	0.54743	8.15182	1.13778
C	-0.86358	7.29216	2.60837
H	-0.87693	8.29053	3.06492
H	-1.90167	6.97391	2.43765
C	2.06629	5.87257	0.74569
H	2.88510	5.36544	1.26855
H	2.44155	6.82638	0.35086
H	1.73623	5.24312	-0.09169
C	-0.70036	6.19740	4.88236
H	-1.50360	5.44908	4.94697
H	-1.11170	7.16673	5.18865
H	0.10712	5.94627	5.57517
C	1.92500	3.08331	2.49845
C	0.99710	2.92701	1.45934
H	0.22852	3.67721	1.27142
C	1.06128	1.79710	0.64288
H	0.34453	1.68036	-0.17018
C	2.04219	0.82050	0.85404
H	2.08816	-0.05324	0.20404
C	2.95493	0.96196	1.89908
H	3.72022	0.20433	2.07266
C	2.89239	2.08439	2.73396
C	3.41828	1.24550	5.44601
C	2.24834	0.47909	5.33101
H	1.69323	0.47302	4.39245
C	1.81660	-0.31043	6.40031
H	0.92275	-0.92656	6.29270
C	2.54527	-0.34068	7.59241
H	2.21310	-0.96584	8.42113
C	3.72343	0.40726	7.70719
H	4.31126	0.36346	8.62436
C	4.15673	1.19871	6.64412
H	5.08475	1.76687	6.73638
C	5.63632	1.90960	3.69545
C	6.10056	0.59687	3.88495
H	5.46839	-0.14598	4.37196
C	7.38034	0.24932	3.45305
H	7.74180	-0.76868	3.59914
C	8.19773	1.20197	2.83709
H	9.19858	0.92532	2.50575
C	7.74016	2.50996	2.65389
H	8.38349	3.25358	2.18374
C	6.46394	2.86806	3.08676
H	6.11074	3.89293	2.95819
N	0.39534	3.16771	5.40859
N	2.04842	4.28770	6.35418
N	0.96761	6.14862	1.66100
N	-0.19812	6.33335	3.52467
P	2.14898	4.55839	3.58770
P	3.96321	2.41606	4.16748

1-frag

C	0.94067	0.47430	0.55568
C	0.54708	2.62306	1.27343

H	-0.27033	3.13170	0.75389
H	1.23498	3.37438	1.65682
C	0.05866	1.64609	2.33024
H	0.65528	1.65920	3.24625
H	-0.98491	1.79556	2.60127
C	1.88952	2.32579	-0.83705
H	2.42410	1.57058	-1.40387
H	2.60118	3.08153	-0.50878
H	1.15051	2.80478	-1.48186
C	-0.33404	-0.85427	2.23981
H	-1.41832	-0.75781	2.30514
H	0.05921	-1.01595	3.24466
H	-0.10544	-1.71534	1.61739
C	3.28698	-0.80864	-0.27592
C	5.53810	-0.91987	-0.76776
H	6.18110	-0.14058	-1.17286
H	5.92307	-1.88331	-1.10786
C	5.36166	-0.84199	0.74151
H	5.83697	-1.66166	1.27780
H	5.72469	0.09475	1.16867
C	3.93430	-0.78719	-2.70121
H	2.91833	-0.49701	-2.94655
H	4.11755	-1.78904	-3.09220
H	4.61868	-0.09675	-3.19015
C	3.28394	-1.00529	2.19772
H	3.15056	-0.01997	2.65074
H	3.91844	-1.59782	2.85230
H	2.32165	-1.50893	2.12518
H	1.39765	-0.35610	-1.70755
H	-1.77654	-0.42292	-2.54017
C	-2.11713	1.22806	-0.74422
C	-1.77672	2.27940	-1.60107
H	-1.29651	2.06732	-2.55078
C	-2.09442	3.58846	-1.27446
H	-1.85476	4.38824	-1.96322
C	-2.75183	3.87040	-0.08289
H	-3.01868	4.88973	0.16174
C	-3.09478	2.83471	0.77555
H	-3.63511	3.04564	1.68964
C	-2.77664	1.52337	0.45067
H	-3.08600	0.71817	1.10903
C	-2.89281	-1.57310	-0.57061
C	-4.24717	-1.24076	-0.66156
H	-4.54515	-0.27984	-1.06305
C	-5.21065	-2.14237	-0.24528
H	-6.25765	-1.88165	-0.32263
C	-4.83713	-3.38122	0.25927
H	-5.59513	-4.08376	0.57881
C	-3.49644	-3.72186	0.34921
H	-3.20599	-4.69018	0.73392
C	-2.52722	-2.81987	-0.06024
H	-1.47879	-3.09375	-0.00504
N	1.24395	1.74337	0.31633
N	0.22887	0.34576	1.66729
N	4.16216	-0.74640	-1.27192
N	3.90098	-0.92212	0.89523
P	1.41807	-0.99671	-0.46325
P	-1.58874	-0.46040	-1.14143

INT1′

Rh	2.71236	7.33965	14.92985
Cl	1.86069	9.63659	15.10710
P	0.71466	6.30418	15.32231
P	2.78428	7.22747	17.23049
N	-1.54819	7.50971	14.09686
N	-1.15659	5.47062	13.32044
C	4.54286	6.46722	14.22212
C	-0.76508	6.42481	14.18331
C	-2.61423	7.31453	13.09643
H	-2.48156	8.05871	12.28456
H	-3.60631	7.47320	13.56509
C	-2.38829	5.87206	12.61350
H	-3.21576	5.18381	12.88629

H	-2.21860	5.81134	11.52034
C	-1.36654	8.82046	14.70101
H	-0.34065	8.94269	15.10469
H	-2.12142	9.00131	15.49285
H	-1.49124	9.58080	13.90478
C	-0.53159	4.19940	12.99742
H	0.54997	4.23484	13.20022
H	-0.67659	4.01781	11.91585
H	-0.97599	3.36282	13.57474
C	0.04198	6.97952	16.90961
C	-1.30535	7.00005	17.30963
H	-2.09406	6.62576	16.63964
C	-1.65534	7.53233	18.56208
H	-2.71246	7.56387	18.86477
C	-0.66270	8.03225	19.42177
H	-0.94290	8.46024	20.39549
C	0.68898	7.98443	19.04175
H	1.47389	8.36282	19.71392
C	1.04336	7.45631	17.79032
C	3.20891	5.57250	17.90811
C	2.28476	4.78274	18.62002
H	1.28194	5.17177	18.84443
C	2.63831	3.48898	19.03472
H	1.90826	2.87726	19.58478
C	3.91379	2.97818	18.74923
H	4.18865	1.96468	19.07706
C	4.84382	3.76756	18.04875
H	5.84992	3.37690	17.83468
C	4.49282	5.05680	17.62625
H	5.22652	5.67516	17.08679
C	3.81826	8.37862	18.20151
C	4.33725	7.98421	19.45513
H	4.14765	6.97137	19.83991
C	5.10459	8.88729	20.20651
H	5.50867	8.57857	21.18216
C	5.36031	10.17711	19.71119
H	5.96689	10.88096	20.30060
C	4.84504	10.56656	18.46310
H	5.04443	11.57623	18.07420
C	4.07461	9.67390	17.70319
H	3.65004	9.97447	16.73243
C	4.81182	7.79360	14.71272
C	3.55166	6.31899	13.19440
H	4.88256	8.64799	14.02057
H	5.43476	7.89931	15.61416
H	4.99434	5.56810	14.66982
C	2.86808	7.47911	12.71662
H	3.23913	5.30499	12.89843
H	3.40667	8.43805	12.68340
H	-1.44468	7.56285	9.45203
C	-0.59492	7.51881	10.15030
C	0.18326	6.35209	10.24664
H	-0.05522	5.47882	9.61947
C	1.29519	6.30993	11.10254
H	1.91998	5.40442	11.12760
C	1.66236	7.44042	11.86839
C	0.86005	8.60534	11.77667
H	1.13048	9.47598	12.39387
C	-0.25412	8.64227	10.92831
H	-0.84470	9.56817	10.84579
C	0.75628	4.49907	15.70221
C	-0.33753	3.82191	16.27704
H	-1.28214	4.35118	16.47098
C	-0.21916	2.46594	16.61709
H	-1.07356	1.93825	17.06666
C	0.99128	1.78582	16.39420
H	1.08255	0.72451	16.66887
C	2.08747	2.46460	15.83754

H	3.04305	1.94279	15.68510
C	1.97218	3.81955	15.49708
H	2.83113	4.37830	15.09960

INT2′

Rh	-0.79332	0.25882	-0.19605
Cl	-2.57275	1.47821	-1.34257
P	-0.16321	-0.45147	-2.21011
P	0.71148	-1.19690	0.54164
N	-0.65982	1.45667	-4.32105
N	1.08115	1.91214	-3.01997
C	-0.46875	1.67190	1.53357
C	-1.21998	-1.66045	-3.08859
C	0.10805	1.02887	-3.30524
C	-0.32992	2.86873	-4.62176
H	-1.09552	3.52146	-4.14833
H	-0.32928	3.04302	-5.71401
C	1.04738	3.04171	-3.97023
H	1.88506	2.94262	-4.69510
H	1.14937	4.00233	-3.43113
C	-1.93358	0.90446	-4.77160
H	-1.83454	-0.17082	-4.99706
H	-2.22316	1.43281	-5.69760
H	-2.70893	1.05107	-3.99096
C	2.07609	1.82300	-1.96774
H	1.59104	1.42191	-1.05151
H	2.43653	2.84515	-1.75739
H	2.93046	1.17663	-2.25404
C	1.50965	-1.20756	-2.13114
C	2.36878	-1.41066	-3.22712
H	2.07361	-1.08473	-4.23663
C	3.62701	-2.00091	-3.02364
H	4.30707	-2.14923	-3.87537
C	4.01931	-2.39484	-1.73214
H	5.00565	-2.85601	-1.57549
C	3.16583	-2.18638	-0.63581
H	3.49172	-2.47014	0.37580
C	1.91112	-1.58088	-0.82755
C	1.77551	-0.73934	1.95460
C	2.87640	0.12183	1.74938
H	3.17219	0.40139	0.72665
C	3.59403	0.62035	2.84572
H	4.45722	1.28221	2.68026
C	3.21151	0.27520	4.15446
H	3.77373	0.66938	5.01381
C	2.11146	-0.57230	4.36308
H	1.80965	-0.84318	5.38565
C	1.39199	-1.07916	3.26863
H	0.53125	-1.74400	3.43587
C	-0.00448	-2.83321	0.95817
C	0.77032	-3.87957	1.50169
H	1.83044	-3.71762	1.74845
C	0.18182	-5.12963	1.74075
H	0.78435	-5.94494	2.16807
C	-1.17539	-5.34106	1.43663
H	-1.63202	-6.32406	1.62578
C	-1.94865	-4.29981	0.89782
H	-3.01136	-4.46240	0.66495
C	-1.36565	-3.04582	0.65936
H	-1.95495	-2.21119	0.24323
C	-1.59071	0.86251	1.78747
C	-0.51854	2.87680	0.73075
H	-2.60162	1.21453	1.52842
H	-1.52281	0.05776	2.53453
H	0.48425	1.44758	2.04119
C	0.57543	3.61841	0.38151
H	-1.50418	3.13406	0.31630

H	1.55138	3.36904	0.83460
H	0.70515	7.37769	-3.49357
C	0.67232	6.61498	-2.70151
C	-0.51275	5.89223	-2.45907
H	-1.40964	6.09113	-3.06586
C	-0.56177	4.92126	-1.45215
H	-1.48233	4.33730	-1.30624
C	0.57555	4.66024	-0.63925
C	1.76013	5.39930	-0.89592
H	2.65025	5.21464	-0.27346
C	1.81002	6.36114	-1.91469
H	2.73855	6.92470	-2.09067
H	-2.96777	-0.99816	-1.97530
C	-2.57972	-1.72074	-2.71034
C	-3.42373	-2.66999	-3.30331
H	-4.48367	-2.71063	-3.01173
C	-2.91903	-3.56615	-4.26100
H	-3.58331	-4.31270	-4.72126
C	-1.56223	-3.51727	-4.62400
H	-1.16174	-4.22700	-5.36291
C	-0.70865	-2.57067	-4.03722
H	0.35463	-2.55868	-4.31228

TS2′

Rh	-0.30416	-0.65057	-0.33528
Cl	-1.45836	-0.44271	-2.51465
P	1.79247	-0.70818	-1.16173
P	0.77025	-1.19888	1.51594
N	1.12003	-2.40080	-3.23684
N	2.00794	-0.52917	-4.02950
C	-2.77873	0.72188	0.49463
C	1.79409	-1.27599	-2.92974
C	0.68295	-2.38959	-4.64538
H	-0.42442	-2.33698	-4.66595
H	1.01454	-3.31189	-5.16426
C	1.33331	-1.10910	-5.20635
H	2.08066	-1.31142	-6.00242
H	0.58669	-0.39156	-5.60357
C	0.55617	-3.34537	-2.28705
H	0.09351	-2.78008	-1.43387
H	1.32677	-4.03710	-1.89325
H	-0.23553	-3.92316	-2.79546
C	2.80679	0.67291	-4.16967
H	2.17172	1.58349	-4.19549
H	3.37849	0.61389	-5.11792
H	3.51572	0.76314	-3.33059
C	2.66908	-2.07426	-0.29585
C	3.72718	-2.84356	-0.80706
H	4.14669	-2.61846	-1.80021
C	4.22976	-3.92080	-0.05422
H	5.04679	-4.53768	-0.45707
C	3.68257	-4.21422	1.20644
H	4.07097	-5.06424	1.78731
C	2.63806	-3.43072	1.73121
H	2.20715	-3.66657	2.71624
C	2.12625	-2.35873	0.98257
C	1.78240	0.11189	2.32834
C	2.86316	-0.19803	3.18140
H	3.07490	-1.24372	3.45065
C	3.68547	0.82673	3.67199
H	4.52927	0.58108	4.33439
C	3.44081	2.16250	3.30617
H	4.09748	2.96254	3.68006
C	2.36774	2.47318	2.45631
H	2.18010	3.51211	2.14930
C	1.53924	1.45118	1.96861
H	0.71159	1.67512	1.27943

C	-0.06040	-2.11094	2.86928
C	-0.05858	-1.66499	4.20462
H	0.48359	-0.74709	4.47561
C	-0.74927	-2.39426	5.18786
H	-0.74506	-2.04263	6.23053
C	-1.43920	-3.56734	4.84339
H	-1.97552	-4.13787	5.61640
C	-1.45045	-4.00976	3.50771
H	-1.99700	-4.92501	3.23448
C	-0.77301	-3.27992	2.52202
H	-0.79945	-3.60351	1.46888
C	-2.15763	-0.67370	0.64653
C	-1.79516	1.77064	0.03235
H	-2.68701	-1.46015	0.07369
H	-2.13616	-0.97607	1.70928
H	-3.23430	1.06049	1.45219
C	-1.43492	2.86458	0.75484
H	-1.46417	1.66288	-1.01546
H	-1.75362	2.93349	1.81035
H	1.46732	7.07468	-1.01462
C	0.89093	6.20768	-0.65935
C	0.31277	5.31326	-1.58043
H	0.43659	5.48247	-2.66106
C	-0.42906	4.21373	-1.13143
H	-0.89172	3.53615	-1.86541
C	-0.62371	3.98053	0.25483
C	-0.04136	4.89522	1.16638
H	-0.19029	4.73778	2.24607
C	0.71233	5.98936	0.71718
H	1.15359	6.68501	1.44693
C	-7.83961	-0.88768	0.29891
C	-6.76418	-1.79458	0.39999
C	-5.44099	-1.40228	0.12658
C	-5.19570	-0.07484	-0.25007
C	-7.62202	0.44689	-0.07735
C	-6.29718	0.81291	-0.33995
C	-3.94395	0.69107	-0.59553
C	-4.46674	2.03863	-0.88598
H	-8.86227	-1.22792	0.51664
H	-6.96557	-2.83367	0.69884
H	-4.61709	-2.12237	0.21127
H	-8.45210	1.16301	-0.16104
H	-3.38652	0.27926	-1.49513
H	-3.89499	2.93295	-1.16163
N	-5.78743	2.07291	-0.72726
H	-6.36635	2.90894	-0.85456
H	5.91034	1.75992	0.27438
C	4.89910	1.83184	-0.15265
C	4.18743	0.65972	-0.45359
H	4.63605	-0.32370	-0.25287
C	2.88403	0.74971	-0.98175
C	2.28818	2.01482	-1.17617
H	1.24179	2.07640	-1.51311
C	3.01126	3.17975	-0.89526
H	2.53583	4.15991	-1.03883
C	4.31712	3.08868	-0.38265
H	4.87464	4.00512	-0.13803

INT4′

Rh	-0.59675	-0.08629	-0.49967
Cl	-0.69943	1.88271	-2.00047
P	1.15688	-0.93925	-1.58844
P	-0.28992	-1.85226	0.76339
N	0.01474	-0.98698	-4.09098
N	2.05404	-0.12901	-4.24338
C	-2.10466	2.06234	1.19088
C	1.17245	-0.75960	-3.43903

C	0.08795	-0.51907	-5.48412
H	-0.79821	0.10195	-5.71982
H	0.10211	-1.38539	-6.18129
C	1.40144	0.28696	-5.50071
H	2.04865	0.04858	-6.36740
H	1.22746	1.38490	-5.48496
C	-1.17565	-1.59107	-3.52613
H	-1.29275	-1.22560	-2.46363
H	-1.11193	-2.69898	-3.51494
H	-2.05308	-1.27356	-4.11820
C	3.44507	0.19411	-3.98983
H	3.57758	1.26652	-3.73350
H	4.03756	-0.02942	-4.89996
H	3.82901	-0.41177	-3.15276
C	1.14725	-2.76967	-1.40530
C	1.75658	-3.69438	-2.26998
H	2.36610	-3.34305	-3.11740
C	1.56939	-5.07257	-2.05626
H	2.03096	-5.80113	-2.73928
C	0.78755	-5.51813	-0.97684
H	0.63444	-6.59654	-0.82064
C	0.19666	-4.59481	-0.09402
H	-0.41894	-4.94449	0.74893
C	0.37420	-3.21844	-0.30557
C	1.11048	-1.64768	1.94921
C	1.82737	-2.74876	2.46377
H	1.51304	-3.77616	2.22569
C	2.96018	-2.53599	3.26435
H	3.51883	-3.39754	3.66057
C	3.38465	-1.22650	3.55078
H	4.27864	-1.06247	4.17128
C	2.67510	-0.12747	3.04020
H	3.00864	0.89780	3.25193
C	1.54286	-0.33707	2.23912
H	0.99341	0.50985	1.80271
C	-1.65032	-2.64560	1.69661
C	-1.57894	-2.91655	3.07623
H	-0.66633	-2.66776	3.63775
C	-2.67671	-3.49996	3.73205
H	-2.61941	-3.70820	4.81101
C	-3.84180	-3.81557	3.01528
H	-4.69871	-4.27335	3.53185
C	-3.91735	-3.53899	1.63773
H	-4.83313	-3.77920	1.07681
C	-2.82986	-2.94696	0.98187
H	-2.88592	-2.70124	-0.09097
C	-2.03140	0.54844	0.93747
C	-0.72538	2.56812	1.52716
H	-3.01911	0.14139	0.63183
H	-1.82204	0.09209	1.92670
H	-2.77738	2.24930	2.05990
C	-0.28601	2.78231	2.78938
H	-0.03087	2.62543	0.67036
H	-1.00593	2.65703	3.61840
H	4.78177	3.74085	4.41157
C	3.75091	3.55619	4.07473
C	3.43327	3.60525	2.70455
H	4.22119	3.83226	1.97090
C	2.12399	3.37031	2.26928
H	1.89475	3.40162	1.19413
C	1.09200	3.08470	3.19708
C	1.42570	3.05003	4.57220
H	0.63672	2.82475	5.30657
C	2.73889	3.27737	5.00771
H	2.97387	3.23704	6.08186
C	-6.29309	2.57214	-2.29469
C	-5.61748	1.35717	-2.03882
C	-4.43548	1.31579	-1.28299

C	-3.94259	2.51642	-0.74464
C	-5.79556	3.78960	-1.81054
C	-4.62333	3.72589	-1.04473
C	-2.69700	2.87230	0.00023
C	-2.79169	4.30760	0.15273
H	-7.21526	2.56599	-2.89370
H	-6.02655	0.42240	-2.44978
H	-3.89601	0.37290	-1.12586
H	-6.29720	4.74332	-2.02887
H	-1.85103	2.70990	-0.85646
H	-2.09522	4.96978	0.68343
N	-3.87820	4.77508	-0.47007
H	-4.12525	5.76575	-0.54859
H	5.53433	-1.35268	0.78601
C	4.81376	-0.67602	0.30403
C	3.70448	-1.21022	-0.37165
H	3.55436	-2.29884	-0.41474
C	2.76338	-0.34290	-0.95937
C	2.92483	1.05750	-0.85626
H	2.14608	1.72339	-1.26259
C	4.05537	1.57837	-0.21600
H	4.19509	2.66742	-0.15518
C	4.99630	0.71395	0.37293
H	5.86602	1.12867	0.90359

TS3′

Rh	-0.10580	-0.00357	-0.15618
Cl	1.02394	1.67686	-1.65005
P	1.24797	-1.50661	-1.10732
P	-0.99849	-1.74481	0.84153
N	0.36411	-1.24967	-3.70494
N	2.52755	-0.76288	-3.59383
C	-1.26912	2.65444	0.95049
C	1.46830	-1.26562	-2.92676
C	0.67673	-0.71560	-5.04118
H	-0.08033	0.03576	-5.33767
H	0.67215	-1.53415	-5.79426
C	2.07174	-0.10517	-4.83455
H	2.77023	-0.31644	-5.66676
H	2.02997	0.99268	-4.66180
C	-0.99133	-1.51842	-3.26247
H	-1.13946	-1.03116	-2.26026
H	-1.19629	-2.60466	-3.17158
H	-1.69454	-1.07630	-3.99117
C	3.83871	-0.43673	-3.05836
H	3.80583	0.51983	-2.49500
H	4.54578	-0.34099	-3.90361
H	4.19430	-1.23796	-2.38955
C	0.51442	-3.18668	-1.01416
C	0.91360	-4.29963	-1.77833
H	1.72848	-4.20357	-2.51263
C	0.25440	-5.52908	-1.61380
H	0.55522	-6.39857	-2.21698
C	-0.78897	-5.64785	-0.67855
H	-1.30229	-6.61230	-0.54905
C	-1.18846	-4.53824	0.08475
H	-2.01833	-4.63465	0.80046
C	-0.54870	-3.29789	-0.08809
C	-0.36503	-2.12498	2.52631
C	-0.95998	-3.08241	3.37429
H	-1.89389	-3.58354	3.07800
C	-0.36458	-3.39108	4.60641
H	-0.83303	-4.13418	5.26912
C	0.82795	-2.75417	4.99389
H	1.29163	-3.00044	5.96095
C	1.42385	-1.80246	4.15012
H	2.35514	-1.30012	4.45124

C	0.82813	-1.48509	2.92003
H	1.27535	-0.73758	2.24466
C	-2.82505	-1.85294	0.96943
C	-3.49801	-1.38036	2.11697
H	-2.92285	-1.05847	2.99729
C	-4.90164	-1.32626	2.13921
H	-5.41742	-0.95708	3.03811
C	-5.64423	-1.74983	1.02481
H	-6.74376	-1.71893	1.05136
C	-4.97829	-2.21804	-0.12236
H	-5.55469	-2.55234	-0.99808
C	-3.57723	-2.25810	-0.15488
H	-3.05992	-2.61149	-1.05939
C	-1.18114	1.15543	1.28848
C	0.07138	3.32044	1.07643
H	-2.20816	0.75700	1.41077
H	-0.68382	1.03520	2.27498
H	-1.99660	3.18131	1.61305
C	0.32562	4.45936	1.76049
H	0.88859	2.80076	0.55234
H	-0.49774	4.95187	2.31058
H	5.13474	6.89642	2.18922
C	4.15792	6.39843	2.09711
C	3.96704	5.38398	1.14009
H	4.79614	5.09289	0.47685
C	2.72545	4.74993	1.01673
H	2.58190	3.97572	0.24689
C	1.64068	5.11290	1.85522
C	1.84467	6.14371	2.80211
H	1.01023	6.44285	3.45607
C	3.08984	6.77769	2.92566
H	3.22688	7.57377	3.67302
C	-5.77086	2.29369	-2.06345
C	-5.33617	1.30229	-1.15857
C	-4.06001	1.34713	-0.56988
C	-3.21755	2.42223	-0.88504
C	-4.93566	3.36686	-2.41304
C	-3.67479	3.39839	-1.80661
C	-1.80455	2.77032	-0.51301
C	-1.57569	4.02891	-1.22081
H	-6.77561	2.22620	-2.50524
H	-6.00621	0.46879	-0.90497
H	-3.73581	0.55511	0.11583
H	-5.25974	4.13907	-3.12557
H	-1.11327	2.00558	-1.05087
H	-0.66725	4.64326	-1.19578
N	-2.63126	4.34040	-1.96932
H	-2.68462	5.15326	-2.59079
H	6.23112	-1.68128	1.72503
C	5.29334	-1.66384	1.14975
C	4.77625	-2.85664	0.61709
H	5.30516	-3.80784	0.77820
C	3.57644	-2.84287	-0.11309
H	3.16589	-3.78317	-0.50783
C	2.89504	-1.62618	-0.31406
C	3.40399	-0.42933	0.24100
H	2.84292	0.50776	0.09652
C	4.60581	-0.45121	0.96124
H	5.00185	0.48212	1.38865

INT5′

Rh	-0.27187	0.48206	-0.58913
Cl	0.99338	1.37058	-2.41791
P	0.96791	-1.49979	-0.28240
P	-1.98844	-0.73762	0.11588
N	1.84650	-1.70918	-2.92185
N	3.55222	-1.55836	-1.51081

C	0.29697	2.77523	1.18403
C	2.22465	-1.72415	-1.63095
C	2.98103	-1.35194	-3.79612
H	2.79198	-0.33773	-4.20495
H	3.06933	-2.07120	-4.63423
C	4.18209	-1.38680	-2.83612
H	4.87152	-2.23633	-3.02827
H	4.77188	-0.44972	-2.84267
C	0.50138	-1.76255	-3.47153
H	-0.23089	-1.33080	-2.76567
H	0.20699	-2.80366	-3.71642
H	0.47485	-1.14230	-4.38569
C	4.38520	-1.57074	-0.31430
H	4.33204	-0.60669	0.22887
H	5.43137	-1.72129	-0.63470
H	4.09628	-2.39386	0.36162
C	-0.25856	-2.82367	-0.64494
C	0.08208	-4.11200	-1.09906
H	1.13995	-4.39049	-1.22507
C	-0.92767	-5.03264	-1.42259
H	-0.65985	-6.03531	-1.78726
C	-2.27780	-4.66622	-1.29306
H	-3.06990	-5.38159	-1.55919
C	-2.62488	-3.38459	-0.83408
H	-3.68378	-3.10070	-0.75251
C	-1.62314	-2.45508	-0.50373
C	-2.24383	-0.99876	1.91610
C	-1.45455	-1.93741	2.61027
H	-0.78415	-2.61285	2.06357
C	-1.52336	-2.02137	4.00827
H	-0.90296	-2.75911	4.53841
C	-2.38273	-1.17072	4.72387
H	-2.43685	-1.23669	5.82069
C	-3.17929	-0.24045	4.03509
H	-3.85944	0.42273	4.59012
C	-3.11153	-0.14982	2.63638
H	-3.73165	0.58308	2.10051
C	-3.64391	-0.25741	-0.49799
C	-4.80308	-0.89014	0.00902
H	-4.71914	-1.67304	0.77755
C	-6.07044	-0.48702	-0.43536
H	-6.96981	-0.97692	-0.03344
C	-6.19141	0.55063	-1.37602
H	-7.18841	0.87296	-1.71155
C	-5.04268	1.18508	-1.87374
H	-5.13196	2.01192	-2.59240
C	-3.77148	0.78227	-1.43956
H	-2.86785	1.29645	-1.80159
C	-0.28050	1.34999	1.30784
C	1.69206	2.68943	0.61398
H	-1.30102	1.38712	1.71876
H	0.33446	0.70386	1.96398
H	0.35550	3.14197	2.23985
C	2.81075	2.38599	1.31182
H	1.74714	2.72696	-0.48378
H	2.76322	2.33858	2.41545
H	7.61852	1.03829	-0.78533
C	6.63650	1.30364	-0.36607
C	5.57143	1.66066	-1.21578
H	5.72616	1.68631	-2.30629
C	4.32073	2.00749	-0.69004
H	3.49363	2.24726	-1.37404
C	4.10933	2.03809	0.71357
C	5.18923	1.67320	1.55406
H	5.04488	1.69063	2.64597
C	6.43554	1.30463	1.02358
H	7.25867	1.03156	1.70090
C	-4.84248	4.10633	0.05015

C	-4.38701	3.40527	1.19377
C	-3.02098	3.21529	1.42887
C	-2.07848	3.71159	0.49744
C	-3.93810	4.65135	-0.86938
C	-2.56609	4.44919	-0.63495
C	-0.63311	3.65280	0.37710
C	-0.31026	4.36938	-0.76780
H	-5.92243	4.24207	-0.10781
H	-5.12285	3.02097	1.91612
H	-2.68733	2.70879	2.34568
H	-4.28938	5.21920	-1.74393
H	-1.28031	1.65705	-0.82998
H	0.66534	4.54243	-1.23200
N	-1.46220	4.84666	-1.36615
H	-1.48963	5.39773	-2.22197
H	3.29202	-2.73317	4.81306
C	2.86466	-2.52110	3.82174
C	2.30138	-3.56339	3.06336
H	2.28963	-4.58968	3.45952
C	1.75049	-3.29966	1.80017
H	1.29749	-4.11694	1.22083
C	1.76649	-1.98395	1.29104
C	2.32124	-0.93828	2.05806
H	2.32988	0.08574	1.65681
C	2.87576	-1.21050	3.31645
H	3.31211	-0.39198	3.90764

TS5′

Rh	-0.26264	0.22342	-0.16337
Cl	0.90962	1.98198	-1.41055
P	1.37413	-1.13617	-1.00423
P	-0.94454	-1.67889	0.75423
N	0.82940	-0.67871	-3.66995
N	2.94106	-0.15592	-3.22180
C	-1.72040	2.78218	0.86414
C	1.80314	-0.68798	-2.74549
C	1.31552	-0.07720	-4.92580
H	0.59715	0.68802	-5.27719
H	1.41019	-0.85954	-5.70972
C	2.66768	0.52305	-4.50620
H	3.48164	0.32651	-5.22968
H	2.60259	1.61667	-4.31825
C	-0.55688	-1.07276	-3.48362
H	-0.89191	-0.73623	-2.47297
H	-0.69341	-2.16932	-3.57539
H	-1.17152	-0.56083	-4.24550
C	4.15083	0.17315	-2.48587
H	4.03310	1.14038	-1.95307
H	4.98702	0.24810	-3.20583
H	4.38351	-0.61612	-1.75251
C	0.71942	-2.84171	-1.14315
C	1.23235	-3.85316	-1.97258
H	2.13595	-3.67338	-2.57589
C	0.56739	-5.09069	-2.04780
H	0.95500	-5.88105	-2.70737
C	-0.59665	-5.31343	-1.29285
H	-1.12110	-6.27762	-1.36759
C	-1.10073	-4.30984	-0.44438
H	-2.01656	-4.48246	0.14161
C	-0.44385	-3.07230	-0.36484
C	0.05855	-2.04990	2.24859
C	0.20135	-3.35732	2.75916
H	-0.36059	-4.19248	2.31453
C	1.08036	-3.59860	3.82552
H	1.18852	-4.61858	4.22364
C	1.83078	-2.54411	4.37586
H	2.52780	-2.74178	5.20386

C	1.69877	-1.24344	3.86398
H	2.29321	-0.41472	4.27508
C	0.81399	-0.99556	2.80510
H	0.72691	0.01967	2.38711
C	-2.70253	-1.95020	1.14266
C	-3.14170	-2.34943	2.42028
H	-2.41102	-2.55391	3.21664
C	-4.51800	-2.47086	2.67546
H	-4.86135	-2.77861	3.67424
C	-5.45171	-2.19194	1.66432
H	-6.52842	-2.28194	1.87142
C	-5.01349	-1.78513	0.39087
H	-5.74145	-1.54760	-0.39848
C	-3.64328	-1.65839	0.12973
H	-3.30155	-1.30507	-0.85561
C	-1.77384	1.25210	0.97571
C	-0.31881	3.27168	1.17764
H	-2.80617	0.87172	0.87895
H	-1.42071	0.91084	1.97152
H	-2.40606	3.16672	1.66279
C	0.41749	2.80672	2.21540
H	0.13691	3.99762	0.48970
H	-0.06594	2.13188	2.94420
H	5.64941	3.70999	3.23995
C	4.58638	3.52426	3.02554
C	4.05926	3.80614	1.75057
H	4.71669	4.20277	0.96166
C	2.70474	3.57944	1.47399
H	2.31039	3.75970	0.46310
C	1.83616	3.07336	2.47411
C	2.38751	2.76950	3.74331
H	1.72766	2.36692	4.52842
C	3.74323	2.99867	4.01994
H	4.14430	2.77183	5.01949
C	-5.74556	2.33075	-2.75194
C	-5.69212	1.75185	-1.45967
C	-4.60622	1.97842	-0.60636
C	-3.53257	2.79265	-1.04577
C	-4.71564	3.16056	-3.21137
C	-3.62383	3.38319	-2.35385
C	-2.27680	3.23401	-0.46576
C	-1.68396	4.05992	-1.40828
H	-6.61573	2.14009	-3.39749
H	-6.53157	1.12982	-1.11367
H	-4.60911	1.54051	0.40232
H	-4.76429	3.62864	-4.20615
H	-1.69930	0.56888	-0.65271
H	-0.71619	4.56849	-1.38455
N	-2.48671	4.14779	-2.53287
H	-2.28256	4.71467	-3.35331
H	5.49371	-1.08937	2.93873
C	4.74640	-1.10900	2.13149
C	4.35137	-2.33739	1.57565
H	4.78474	-3.27750	1.94744
C	3.39298	-2.37410	0.55032
H	3.06689	-3.33751	0.13237
C	2.83132	-1.16711	0.08771
C	3.20532	0.06848	0.66890
H	2.71897	1.00136	0.34024
C	4.17505	0.09336	1.67759
H	4.45755	1.05671	2.12646

INT6′

h	-0.79682	-0.58985	0.16332
Cl	-2.80985	-1.89110	0.50971
P	-0.88719	-1.01332	-2.01716
P	1.34935	-0.13864	-0.26077

N	-1.29277	-3.78424	-2.07381
N	-3.13472	-2.65868	-2.60628
C	-0.20613	-0.54198	3.36627
C	-1.82597	-2.57893	-2.32551
C	-2.30474	-4.84391	-2.24538
H	-2.30936	-5.50839	-1.35958
H	-2.06475	-5.45555	-3.14124
C	-3.61149	-4.04309	-2.39767
H	-4.23116	-4.37666	-3.25216
H	-4.22769	-4.06010	-1.47404
C	0.02484	-4.05363	-1.52046
H	0.32562	-3.21626	-0.85920
H	0.79343	-4.19361	-2.30697
H	-0.03987	-4.97201	-0.90773
C	-4.10303	-1.56655	-2.62149
H	-3.70241	-0.68359	-2.09592
H	-5.00178	-1.90312	-2.07093
H	-4.38680	-1.28997	-3.65625
C	0.77739	-1.31017	-2.73943
C	1.05280	-1.86736	-4.00203
H	0.23653	-2.22345	-4.64755
C	2.38370	-1.97679	-4.43196
H	2.60782	-2.42337	-5.41201
C	3.43124	-1.51252	-3.61413
H	4.47296	-1.59611	-3.95740
C	3.15489	-0.94567	-2.36076
H	3.97762	-0.59025	-1.72378
C	1.82399	-0.84842	-1.91486
C	1.87468	1.61170	-0.41272
C	1.62993	2.28328	-1.62966
H	1.25029	1.72863	-2.50108
C	1.86390	3.66222	-1.73221
H	1.67269	4.17663	-2.68564
C	2.33950	4.38298	-0.62270
H	2.52286	5.46455	-0.70553
C	2.57732	3.71933	0.59280
H	2.94167	4.27339	1.47052
C	2.34252	2.33960	0.70334
H	2.51944	1.84552	1.67048
C	2.56145	-0.95029	0.85212
C	3.88452	-0.48751	1.01400
H	4.21942	0.42814	0.50529
C	4.77037	-1.18229	1.85251
H	5.79759	-0.81196	1.98588
C	4.34386	-2.33646	2.53136
H	5.03735	-2.86821	3.19946
C	3.03088	-2.80770	2.36170
H	2.69256	-3.70771	2.89601
C	2.14266	-2.11885	1.52305
H	1.10229	-2.46185	1.39649
C	-0.73848	-1.87208	3.91330
C	-1.13026	0.02884	2.29684
H	-1.71993	-1.73351	4.41097
H	-0.03904	-2.30283	4.65567
H	0.77951	-0.73442	2.90184
C	-0.78083	1.15505	1.53298
H	-2.19872	-0.20706	2.42973
H	0.22132	1.58072	1.69923
H	-4.04747	4.55219	-1.11374
C	-3.38956	3.85491	-0.57373
C	-3.89781	2.63280	-0.09272
H	-4.95441	2.37453	-0.25954
C	-3.07180	1.74409	0.60456
H	-3.47479	0.78253	0.95426
C	-1.70522	2.05795	0.82729
C	-1.20514	3.28926	0.33590
H	-0.15017	3.54543	0.50697
C	-2.04019	4.17927	-0.35441

H	-1.63301	5.13447	-0.71882
C	3.38622	2.91139	5.41411
C	3.61955	1.89422	4.45282
C	2.59258	1.03355	4.05078
C	1.30388	1.19604	4.60795
C	2.12665	3.08089	6.00343
C	1.09388	2.21784	5.59372
C	0.04591	0.51348	4.41827
C	-0.86210	1.11930	5.27844
H	4.21341	3.57150	5.71464
H	4.62789	1.77356	4.02873
H	2.78957	0.22747	3.33004
H	1.95576	3.86110	6.76008
H	-0.89043	-2.59886	3.08940
H	-1.92698	0.91405	5.43613
N	-0.23134	2.13582	5.98040
H	-0.67439	2.72086	6.68677
H	-1.47290	1.78233	-1.70172
C	-1.71446	1.53145	-2.74477
C	-2.13845	2.52630	-3.64049
H	-2.22594	3.56265	-3.28548
C	-2.45502	2.19497	-4.96684
H	-2.79179	2.97574	-5.66498
C	-2.34606	0.86247	-5.40696
H	-2.59688	0.60168	-6.44595
C	-1.91295	-0.13511	-4.52344
H	-1.83385	-1.17538	-4.87423
C	-1.60105	0.20017	-3.18748

References

[1] Basra, S.; Vries, J. G. de; Hyett, D, J.; Harrison, G.; Heslop, K. M.; Orpen, A. G.; Pringle, P. G.; Luehe, K. *J. Am. Chem. Soc* **1985**, *107*, 4491.
[2] Weiss, R.; Wagner, K. G.; Priesner, C.; Macheleid, J. *J. Am. Chem. Soc* **1985**, *107*, 4491.
[3] Cereghetti, M.; Arnold, W.; Broger, E. A.; Rageot, A. *Tetrahedron Lett.* **1996**, *37*, 5347.
[4] Mancino, G.; Ferguson, A. J.; Beeby, A.; Long, N. J.; Jones, T. S. *J. Am. Chem. Soc.* **2005***, 127*, 524.
[5] a) Becke, A. D. *Phys. Rev. A*, **1998**, *38*, 3098-3100. b) Perdew, J. P. *Phys. Rev. B*, **1986**, *33*, 8822-8824.
[6] Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241.
[7] a) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104. b) Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comput. Chem.* **2011**, *32*, 1456-1465.
[8] a) Schäfer, A.; Horn, H.; Ahlrichs, R. *J. Chem. Phys.* **1992**, *97*, 2571-2577. b) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305. c) Weigend, F. *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057-1065.
[9] Andrae, D.; Häussermann, U.; Dolg, M.; Stoll, H.; *Theor. Chim. Acta* **1990**, *77*, 123-141.
[10] a) Eichkorn, K.; Treutler, O.; Öhm, H.; Häser, M.; Ahlrichs, R. *Chem. Phys. Lett.* **1995**, *240*, 283-290. b) Eichkorn, K. Weigend, F.; Treutler, O.; Ahlrichs, R. *Chem. Phys. Lett.* **1995**, *242*, 652-660.
[11] Sierka, M.; Hogekamp, A.; Ahlrichs, R. *J. Chem. Phys.* **2003**, *118*, 9136-9148.
[12] Ribeiro, R. F.; Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2011**, *115*, 14556-14562.
[13] Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995-2001.
[14] a) Ahlrichs, R.; Bär, M.; Häser, M.; Horn, H.; Kölmel, C. *Chem. Phys. Lett.* **1989**, *162*, 165-169. b) TURBOMOLE V6.4 2012, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, **1989-2007**, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com
[15] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.
[16] G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders, T. Ziegler, *J. Comput. Chem*. **2001**, *22*, 931 – 967.
[17] a) Clementi E.; Roetti C. *At. Nucl. Data Tables* **1974**, *14*, 177 – 478. b) McLean, A. D; Mclean, R. S. *At. Nucl. Data Tables* **1981**, *26*, 197 – 381. c) Snijders, J. G; Vernooijs, P.; Baerends, E. J. *At. Nucl. Data Tables* **1981**, *26*, 483 – 581. d) Chong, D. P.; Lenthe, E. V.; Gisbergen, S. V.; Baerends, E. J. *J. Comput. Chem.* **2004**, *25*, 1030 – 1036.
[18] van Lenthe, E.; Baerends, E. J.; Snijders, J. G. *J. Chem. Phys.* **1994**, *101*, 9783 – 9792.