Electronic Supplementary Material (ESI) for Chemical Communications.

Regulating Iminophosphoranes P=N bonds Reactivity Through Geometric Constraints with Cage-Shaped Triarylphosphines

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Contents

1. General experimental procedures.

1.1. General information

All the catalytic and stoichiometric reactions have been carried out under argon or nitrogen atmosphere using a standard Schlenk line and glove box technique in oven dried glassware. Reaction temperatures are disclosed as the temperature of the bath surrounding the vessel unless otherwise mentioned.

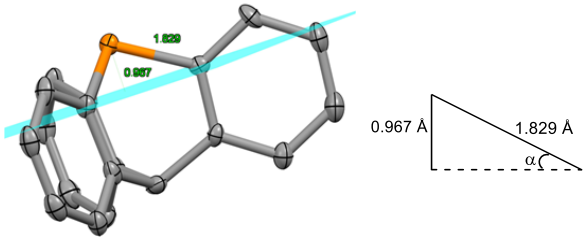
Chemicals and Materials. 4Å Molecular sieves were dried at 400 °C under high vacuum for 3 days and stored in a glove box. Diethylether, tetrahydrofuran, toluene and dichloromethane were dried with an MBraun solvent purification system and stored under argon. CD_2Cl_2 was dried over preactivated 4Å molecular sieves and stored in a glovebox, all others solvents were dried over CaH_2, distilled and stored over preactivated 4Å molecular sieves in a glove box prior to use. Others reagents and chemicals were purchased from Sigma-Aldrich, Alfa Aesar, TCI and Fluorochem and used without further purification.

Analytical: NMR spectra were recorded on 400 or 500 MHz NMR JEOL spectrometers. The observed signals are reported in parts per million (ppm) relative to the residual signal of the non-deuterated solvent for ^{1}H and ^{13}C NMR spectra. The following abbreviations are used to describe multiplicities s = singlet, d = doublet, t = triplet, q = quartet, quin = quintuplet, br = broad, m = multiplet. The external references considered as 0.0 ppm are borontrifluoride etherate ($BF_3{\cdot}Et_2O$) for ^{11}B NMR, trichloromonofluoromethane ($CFCl_3$) for ^{19}F NMR and H_3PO_4 (85%) for ^{31}P NMR. Melting points were determined on a Büchi B-545 device and are not corrected. Infrared spectra were recorded on a PerkinElmer FT-IR Spectrometer. MALDI ionization was performed on a WATERS QTOF Premier mass spectrometer.

Chromatography. Flash chromatography was performed using silica gel Silica Flash® 40-63 micron (230-400 mesh) from Sigma-Aldrich. TLC detection was accomplished by irradiation with a UV lamp at 265 or 313 nm and Iodine strain.

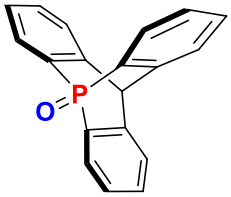
2. **Calculation of pyramidization angle α :** The pyramidization angle α was calculated according to the following procedure. In the crystallographic structure of the phosphines, a hypothetical plane containing three C_{sp2} carbon atoms (connected to P atom) was drawn. The distance between phosphorus and the plane was measured. The P - C_{sp2} bond length can also be measured easily. Then the pyramidization angle α can be easily determined by inverse trigonometric sine function (asin) according to the diagram below or can be directly

determined via placing a plan going through the carbon atoms attached to P using the Mercury software.



Sin α = (0.967/ 1.829) = 0.5, α = $\sin^{-1}(0.5)$ = 0.52 rad, α = 29.8 º

3. Synthesis and Characterization of compounds



6

Compound **6** was prepared according to the described procedure. 9-phosphatriptycene **5** (1.0 g, 3.6 mmol) was dissolved in DCM (20 mL) in a 100 mL flask and a solution of H_2O_2 in water (40 mL, 3%) was added, then the reaction mixture was stirred at room temperature for 1 h. After 1 h later; the layers were separated, and the organic phase was dried over Na_2SO_4. Evaporation of the organic solvent produced pure 9-phosphatriptycene oxide **6** (0.985 g, 95%) as colorless needles.

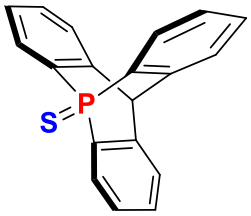
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.04 – 7.97 (m, 3H), 7.54 – 7.47 (m, 3H), 7.29 – 7.20 (m, 6H), 5.42 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 147.59 (d, *J* = 7.0 Hz), 133.40 (d, *J* = 96.2 Hz), 130.05 (d, *J* = 1.8 Hz), 128.38 (d, *J* = 6.0 Hz), 126.23 (d, *J* = 12.1 Hz), 125.51 (d), 53.99 (d, *J* = 18.6 Hz).

^{31}P NMR (202 MHz, Chloroform-*d*) δ 7.38.

IR (neat, ATR): $\tilde{\nu}$ / cm^{-1} = 1589, 1440, 1282, 1232 ($\nu_{P=O,}$ str), 1178, 1130, 1064, 857, 762, 704, 612, 556.

M.p.: 284-286 °C



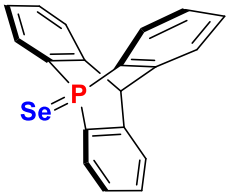
7

Compound **7** was prepared by slightly modifying procedure described in relative literature.[1] A suspension of **5** (46 mg, 0.12 mmol) and Lawesson's reagent (234.5 mg, 0.58 mmol) in toluene (10 mL) was refluxed overnight. The solvents were removed under reduced pressure and the resulting crude was purified by column chromatography giving **7** as a white solid (29 mg, 0.096 mmol, 80%). The corresponding crystal suitable for X-ray structure analysis was obtained by slow evaporation of a saturated solution of **7** in $CHCl_3$/ EtOH.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.07 – 8.00 (m, 3H), 7.56 – 7.52 (m, 3H), 7.31 – 7.23 (m, 6H), 5.54 (s, 1H).
^{13}C NMR (126 MHz, Chloroform-*d*) δ 146.98 (d, J = 4.1 Hz), 133.81 (d, J = 78.8 Hz), 130.06 (d, J = 2.4 Hz), 128.70 (d, J = 9.1 Hz), 126.26 (d, J = 13.1 Hz), 125.31 (d, J = 7.8 Hz), 54.82 (d, J = 16.3 Hz).
^{31}P NMR (202 MHz, Chloroform-*d*) δ 12.71.

IR (neat, ATR): $\tilde{\nu}$ / cm^{-1} = 3059, 2924, 2854, 1586, 1442, 1274, 1135, 1071, 1057, 1021, 956, 860 ($\nu_{P=S,}$ str), 850, 745, 696, 678, 637, 610, 543, 462.

M.p.: 316-318 °C



8

Compound **8** was prepared by slightly modifying procedure described in relative literature.[1] In a pre-dried 25ml Schlenk flask **5**(46 mg, 0.17 mmol) and Se powder (110 mg, 1.4 mmol) was added in Ar atmosphere. Then $CDCl_3$ (4.0 ml) was added, and the resulting mixture was refluxed for 3 h. Then the residual elemental selenium was filtered off and the solvent was removed under reduced pressure to obtain **8** as white solid (47 mg, 0.13 mmol, 76%).

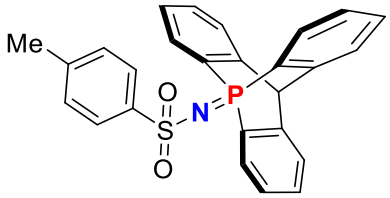
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.06 – 8.00 (m, 3H), 7.56 – 7.52 (m, 3H), 7.31 (t, *J* = 1.4 Hz, 1H), 7.30 (t, *J* = 1.4 Hz, 4H), 7.29 – 7.26 (m, 3H), 7.25 (dd, *J* = 3.1, 1.2 Hz, 1H), 5.58 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 146.75 (d, *J* = 2.3 Hz), 132.80 (d, *J* = 70.4 Hz), 130.21 (d, *J* = 2.1 Hz), 129.63 (d, *J* = 10.6 Hz), 126.27 (d, *J* = 13.4 Hz), 125.20 (d, *J* = 7.2 Hz), 55.54 (d, *J* = 15.1 Hz).

^{31}P NMR (202 MHz, Chloroform-*d*) δ 4.52 (s, $^{1}J_{SeP}$ = 821.7 Hz{sattelite}).

IR (neat, ATR): $\tilde{\nu}$ / cm^{-1} = 2922, 2852, 1587, 1449, 1378, 1273, 1232, 1179, 1131, 1068, 1059, 1021, 857, 847, 763, 748, 696, 611 ($\nu_{P=Se,}$ str), 584, 573, 558, 539.

M.p.: 76-78 °C(dec)



9

Compound **9** was prepared by following the discussed procedure. 9-phosphatriptycene **5** (100 mg, 0.36 mmol) was dissolved in Et_2O-DCM (2 mL) in a 25 mL flask and a solution of *p*-toluenesulfonyl azide (78 mg in 1 mL DCM, 0.40 mmol) was added, then the reaction mixture was stirred at 40 °C for 4 h. The solution was evaporated in vacuo and the residue was washed with MeOH (5 mL). The mixture was filtered to afford **9** as a white solid (146 mg, 0.33 mmol, 91%). The corresponding crystal suitable for X-ray structure analysis was obtained by slow evaporation of a saturated solution of **9** in EtOAc.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.28 – 8.10 (m, 4H), 7.64 – 7.48 (m, 3H), 7.43 – 7.14 (m, 9H), 5.53 (s, 1H), 2.46 (s, 3H).

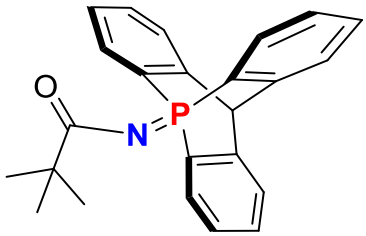
^{13}C NMR (126 MHz, Chloroform-*d*) δ 147.12 (d, J = 7.5 Hz), 143.03 (d, J = 6.5 Hz), 141.82, 130.78 (d, J = 2.5 Hz), 130.34, 130.11 (d, J = 5.9 Hz), 129.57, 129.41, 126.62 (d, J = 12.7 Hz), 126.16, 125.65 (d, J = 9.5 Hz), 54.61 (d, J = 19.8 Hz), 21.65.

^{31}P NMR (161 MHz, Chloroform-*d*) δ -7.51.

IR (neat, ATR): $\tilde{\nu}$ / cm^{-1} = 1588, 1444, 1272, 1197, 1178, 1143, 1091, 1064, 892, 864, 850, 819, 782, 759, 702, 691, 666, 610, 577, 556, 542, 513.

HRMS (ESI$^+$): Calcd. for $C_{26}H_{21}O_2NPS$ $[M + H]^+$: 442.10251, found: 442.10250.

M.p.: 347-348 °C



10

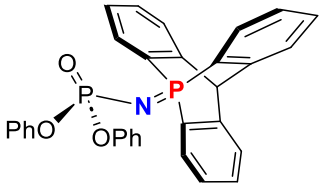
Compound **10** was prepared according to the procedure described in the literature.[2] Pivalic anhydride (2.0 mL, 9.9 mmol) and sodium azide (0.77 g, 11.8 mmol) were stirred in dry, degassed acetone (100 mL) for 10 min. 9-phosphatriptycene **5** (2.7 g, 9.9 mmol) was added in one portion and the resulting solution was stirred at room temperature for 72 h. The solvent was removed under reduced pressure and the solid extracted into dichloromethane (40 mL) and filtered. Diethyl ether (60 mL) was added, and the solution was stored at 25 ° C. Compound **10** crystallized as white crystals (1.7 g, 4.6 mmol, 46%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 12.0, 7.2 Hz, 3H), 7.58 – 7.48 (m, 3H), 7.32 – 7.16 (m, 6H), 5.53 (s, 1H), 1.54 (d, *J* = 0.9 Hz, 9H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 192.82 (d, *J* = 11.4 Hz), 147.46 (d, *J* = 5.6 Hz), 130.75 (d, *J* = 90.8 Hz), 130.10 (d, *J* = 1.3 Hz), 129.99 (d, *J* = 6.4 Hz), 126.21 (d, *J* = 12.0 Hz), 125.48 (d, *J* = 8.4 Hz), 54.96 (d, *J* = 17.6 Hz), 41.92 (d, *J* = 17.4 Hz), 29.13.

^{31}P NMR (161 MHz, Chloroform-*d*) δ -5.54.

HRMS (ESI^{+}): Calcd. for $C_{24}H_{23}ONP$ $[M + H]^{+}$: 372.15118, found: 372.15088.



11

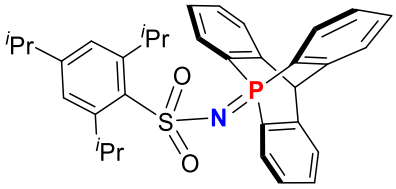
Compound **11** was prepared by following the discussed procedure. 9-phosphatriptycene (100 mg, 0.36 mmol) was dissolved in Et_2O-DCM (2 mL) in a 25 mL flask and a solution of diphenylphosphoryl azide (110 mg in 1 mL DCM, 0.40 mmol) was added, then the reaction mixture was stirred at 40 °C for 4h. The solution was evaporated in vacuo and the residue was washed with MeOH (5 mL). The mixture was filtered to afford **11** as a white solid (156 mg, 0.3 mmol, 82%). The corresponding crystal suitable for X-ray structure analysis was obtained by slow evaporation of a saturated solution of **11** in EtOAc.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (dd, *J* = 13.4, 7.0 Hz, 3H), 7.51 (dd, *J* = 6.7, 6.0 Hz, 3H), 7.46 (ddd, *J* = 6.5, 2.2, 1.1 Hz, 4H), 7.34 (t, *J* = 7.8 Hz, 4H), 7.27 (tt, *J* = 7.5, 1.1 Hz, 2H), 7.21 – 7.12 (m, 6H), 5.47 (s, 1H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 152.61 (d, *J* = 7.7 Hz), 147.17 (d, *J* = 7.8 Hz), 131.23 (dd, *J* = 99.7, 3.3 Hz), 130.48 (d, *J* = 1.5 Hz), 129.59, 129.36 (d, *J* = 5.8 Hz), 126.51 (d, *J* = 12.7 Hz), 125.50 (d, *J* = 9.5 Hz), 124.28, 121.01 (d, *J* = 4.9 Hz), 54.32 (d, *J* = 20.1 Hz).

^{31}P NMR (161 MHz, Chloroform-*d*) δ -5.20 (d, *J* = 36.9 Hz), -10.63 (d, *J* = 37.0 Hz).

HRMS (ESI$^+$): Calcd. for $C_{31}H_{24}O_3NP_2$ $[M + H]^+$: 520.12259, found: 520.12186.



12

Compound **12** was prepared by following the discussed procedure. 9-phosphatriptycene **5** (100 mg, 0.36 mmol) was dissolved in Et_2O-DCM (2 mL) in a 25 mL flask and 2,4,6-triisopropylbenzenesilfonyl azide (10-15% water) (0.113gm, 0.40 mmol) was added, then the reaction mixture was stirred at 40 °C for 4 h. The solution was evaporated in vacuo and the residue was washed with MeOH (5 mL). The mixture was filtered to afford **12** as a white solid (183 mg, 0.33 mmol, 91%). The corresponding crystal suitable for X-ray structure analysis was obtained by slow evaporation of a saturated solution of **12** in EtOAc.

^{1}H NMR (400 MHz, Methylene Chloride-d_2) δ 8.02 (dd, J = 13.2, 7.3 Hz, 3H), 7.67 – 7.54 (m, 3H), 7.33 (td, J = 7.5, 1.1 Hz, 3H), 7.30 – 7.19 (m, 5H), 5.59 (s, 1H), 4.91 – 4.78 (m, 2H), 3.01 – 2.89 (m, 1H), 1.35 (d, J = 6.8 Hz, 12H), 1.30 (d, J = 6.9 Hz, 6H).

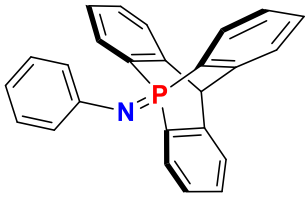
^{13}C NMR (126 MHz, Methylene Chloride-d_2) δ 151.88, 148.87, 147.73 (d, J = 7.3 Hz), 131.19 (d, J = 2.0 Hz), 131.13, 130.36, 130.27 (d, J = 5.8 Hz), 126.84 (d, J = 12.5 Hz), 126.21 (d, J = 9.3 Hz), 123.93, 54.89 (d, J = 19.3 Hz), 34.76, 29.89, 25.18, 24.09.

^{31}P NMR (161 MHz, Methylene Chloride-d_2) δ -7.61.

HRMS (ESI$^+$): Calcd. for $C_{34}H_{37}O_2NPS$ $[M + H]^+$: 554.22771, found: 554.22780.

IR (neat, ATR): $\tilde{\nu}$ / cm^{-1} = 2957, 2924, 2865, 1599, 1588, 1448, 1441, 1384, 1363, 1276, 1249, 1190, 1167, 1126, 1061, 783, 760, 753, 711, 701, 691, 674, 611, 590, 555, 535,488.

M.p.: 285-287 °C



13

Compound **13** was prepared by the procedure described below. 9-phosphatriptycene **5** (100 mg, 0.36 mmol) was dissolved in dry Et_2O (2 mL) in a 25 mL flask and a solution of azidobenzene (0.8M in *t*-butyl methyl ether) 0.40 mmol was added, then the reaction mixture was refluxed for 2 h. After 1 h, white precipitate started to appear. After an additional 1 h of stirring, the mixture was filtered through sintered funnel and washed with distilled Et_2O (5 mL) to afford **13** as a white solid (98 mg, 0.27 mmol, 74%). The corresponding crystal suitable for X-ray structure analysis was obtained by slow evaporation of a saturated solution of **13** in Et_2O.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.03 – 7.95 (m, 3H), 7.55 (dd, *J* = 7.4, 4.5 Hz, 3H), 7.28 (tdd, *J* = 3.7, 2.4, 1.2 Hz, 4H), 7.26 – 7.24 (m, 1H), 7.23 – 7.17 (m, 5H), 6.85 (tt, *J* = 7.1, 1.3 Hz, 1H), 5.48 (s, 1H).

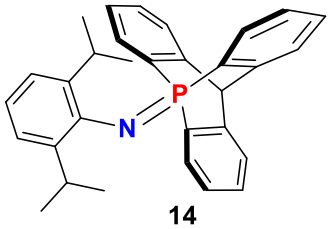
^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.60, 147.87 (d, *J* = 6.0 Hz), 132.69, 131.97, 129.93 (d, *J* = 2.3 Hz), 129.70 (d, *J* = 6.0 Hz), 129.08 (d, *J* = 2.3 Hz), 126.11 (d, *J* = 11.8 Hz), 125.60 (d, *J* = 8.3 Hz), 123.34 (d, *J* = 20.1 Hz), 118.26, 54.51 (d, *J* = 17.5 Hz).

^{31}P NMR (202 MHz, Chloroform-*d*) δ -20.38.

HRMS (ESI$^+$): Calcd. for $C_{25}H_{18}NP$ $[M + H]^+$: 364.1250, found: 364.1272.

IR (neat, ATR): $\tilde{\nu}$ / cm^{-1} = 1588, 1481, 1448, 1327, 1277, 1264, 1173, 1143, 1096, 1064, 1040, 1017, 859, 758, 750, 708, 697, 612, 570, 548.

M.p.: 240-242 °C (dec)



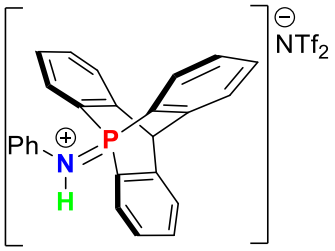
14

Compound **14** was prepared by the procedure described below. 9-phosphatriptycene **5** (50 mg, 0.18 mmol) was dissolved in toluene (4 mL) in a 25 mL flask and 0.2 mmol of 2,6-diisopropylphenyl azide was added, then the reaction mixture was heated at 80 °C overnight. Then the solvent was evaporated at low pressure to to afford **14** as a white solid (68.5 mg, 0.15 mmol, 85%). The corresponding crystal suitable for X-ray structure analysis was obtained by slow evaporation of a saturated solution of **14** in CH_2Cl_2.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.95 (dd, *J* = 11.6, 7.3 Hz, 3H), 7.51 (dd, *J* = 7.1, 5.1 Hz, 3H), 7.27 (s, 1H), 7.24 (d, *J* = 7.5 Hz, 3H), 7.21 – 7.16 (m, 5H), 5.39 (s, 1H), 3.93 (hept, *J* = 6.8 Hz, 2H), 1.21 (d, *J* = 6.8 Hz, 12H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 147.79 (d, *J* = 6.8 Hz), 143.35, 142.93 (d, *J* = 7.3 Hz), 135.15 (d, *J* = 93.5 Hz), 129.69 – 129.57 (m), 129.32 (d, *J* = 5.0 Hz), 126.02 (d, *J* = 11.4 Hz), 125.47 (d, *J* = 8.6 Hz), 122.83, 120.38 – 120.04 (m), 54.33 (d, *J* = 17.6 Hz), 28.92, 24.12.

^{31}P NMR (202 MHz, Chloroform-*d*) δ -33.50.



15

Compound **15** was prepared by the procedure described below. An NMR tube was charged with triflimidic acid ($NHTf_2$) (7.9 mg, 2.8×10^{-2} mmol), 9-phospatriptycene imine **13** (10.2 mg, 2.8×10^{-2} mmol), and 0.6 mL of $CDCl_3$ inside a glove box. After measurements of the NMR spectra, the solvent was slowly evaporated inside glove box to get the crystals suitable for X-ray analysis (16.5 mg, 2.5×10^{-2} mmol, 91%).

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.40 (d, *J* = 12.3 Hz, 1H), 7.95 – 7.88 (m, 3H), 7.77 (d, *J* = 6.9 Hz, 3H), 7.49 – 7.38 (m, 7H), 7.33 – 7.24 (m, 4H), 5.91 (s, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.95 (d, J = 7.7 Hz), 136.70, 132.86, 130.36, 129.68, 127.44 (d, J = 13.1 Hz), 127.05 (d, J = 10.1 Hz), 125.55, 124.12, 123.16, 120.31 (d, J = 7.5 Hz), 54.80 (d, J = 22.9 Hz).

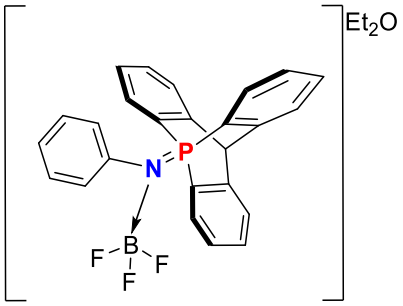
^{31}P NMR (202 MHz, Chloroform-*d*) δ 10.66.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -78.51.

HRMS (ESI^{+}): Calcd. for $C_{25}H_{19}NP^{+}$ $[M]^{+}$: 364.1250, found: 364.1277.

IR (neat, ATR): $\tilde{\nu}$ / cm^{-1} = 3214, 1603, 1589, 1499, 1446, 1413, 1351, 1182, 1135, 1054, 989, 747, 711, 610, 570, 545.

M.p.: 187-188 °C (dec)



16

Compound **16** was prepared by the procedure described below. An NMR tube was charged with 9-phospatriptycene imine **13** (10.2 mg, 2.8×10^{-2} mmol), Boron trifluoride ethyl etherate (2.8×10^{-2} mmol, 3.45µL) and 0.6 mL of CD_2Cl_2 inside a glove box. After measurements of the NMR spectra, the solvent was slowly evaporated inside glove box to get the crystals suitable for X-ray analysis (16.5 mg, 2.5×10^{-2} mmol, 85%).

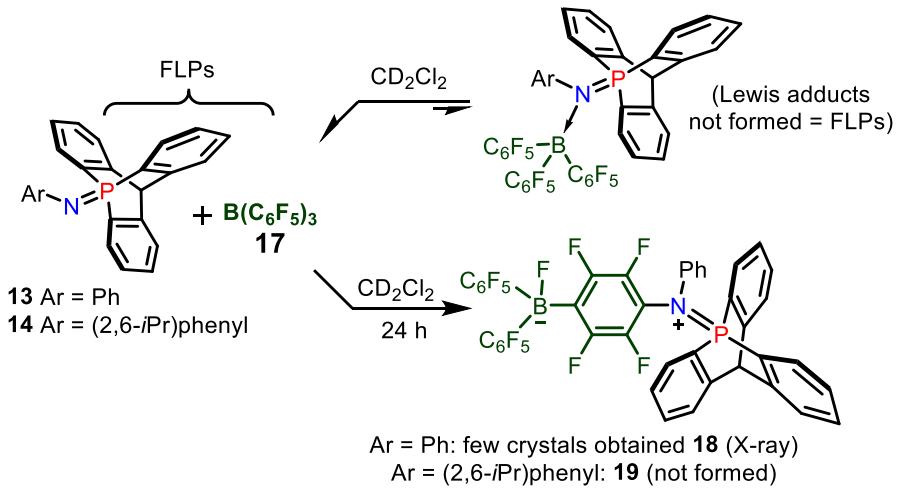
^{1}H NMR (400 MHz, Methylene Chloride-d_2) δ 7.70 – 7.62 (m, 4H), 7.58 (d, J = 6.7 Hz, 2H), 7.52 – 7.31 (m, 8H), 7.23 (s, 3H), 5.68 (s, 1H).

^{13}C NMR (101 MHz, Methylene Chloride-d_2) δ 147.64 (d, J = 6.0 Hz), 141.26 – 141.11 (m), 131.75, 130.85 (d, J = 5.5 Hz), 130.03, 129.70 (d, J = 5.4 Hz), 127.61, 127.39, 127.14 (d, J = 12.3 Hz), 126.56 (d, J = 9.6 Hz), 55.56 (d, J = 20.1 Hz).

^{31}P NMR (202 MHz, Methylene Chloride-d_2) δ 9.23 (m).

^{11}B NMR (160 MHz, Methylene Chloride-d_2) δ -0.92.

^{19}F NMR (471 MHz, Methylene Chloride-d_2) δ -139.87 (m, J = 18.2 Hz)



The frustrated Lewis pair consisting in the combination of **13** and **17** was prepared by the procedure described below. An NMR tube was charged with trispentafluorophenylborane (14.3 mg, 2.8×10^{-2} mmol), 9-phospatriptycene imine **13** (10.2 mg, 2.8×10^{-2} mmol), and 0.6 mL of $CDCl_3$ inside a glove box. A slight broadening of the peaks of both components indicated the presence of an encounter complex or a frustrated Lewis pair, but the absence of shielding or deshielding or of new signals suggested that no Lewis adduct was formed under these conditions. After measurement of NMR spectra, the mixture was kept inside glove box for one day, crystals of compound **18** were obtained among other decomposition products such as 9-phosphatriptycene oxide. Thus, the deactivation of the FLP occurs via S_NAr reaction of the nitrogen atom of the 9-phospatriptycene imine **13** at the para position of one C_6F_5 rings of $B(C_6F_5)_3$, which was not observed in the case of **14** since of larger steric hindrance around it's nitrogen atom which preclude such type of S_NAr reaction.

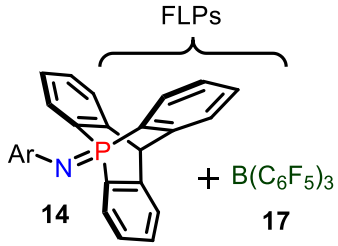
NMR data for the FLP of **13** + **17**

^{1}H NMR (500 MHz, Chloroform -*d*) δ 8.00 – 7.92 (m, 3H), 7.62 – 7.54 (m, 3H), 7.32 – 7.27 (m, 5H), 7.26 – 7.21 (m, 2H), 7.20 – 7.14 (m, 3H), 6.94 – 6.88 (m, 1H), 5.52 (s, 1H).

^{31}P NMR (202 MHz, Chloroform -*d*) δ -17.40.

^{11}B NMR (160 MHz, Chloroform -*d*) δ 55.87.

^{19}F NMR (471 MHz, Chloroform -*d*) δ -127.62, -142.63, -159.91.



Ar = 2,6-diisopropylphenyl

The frustrated Lewis pair between **14** + **17** was prepared by the procedure described below. An NMR tube was charged with trispentafluorophenylborane **17** (14.3 mg, 2.8 × 10^{-2} mmol), 9-phospatriptycene imine **14** (12.52 mg, 2.8 × 10^{-2} mmol), and 0.6 mL of CD_2Cl_2 inside a glove box. The shifts in heteroatom NMR suggested the possible formation of frustrated Lewis pair. Crystal suitable for X-ray analysis were obtained by evaporation of the solvent inside the glove box.

NMR data for the FLP of **14** + **17**

^{1}H NMR (400 MHz, Methylene Chloride-d_2) δ 7.85 (dd, J = 11.8, 7.4 Hz, 3H), 7.63 – 7.55 (m, 3H), 7.32 (t, J = 7.5 Hz, 3H), 7.26 – 7.15 (m, 5H), 7.08 (q, J = 9.9, 6.7 Hz, 1H), 5.52 (s, 1H), 3.83 (hept, J = 6.8 Hz, 2H), 1.19 (d, J = 6.8 Hz, 12H).

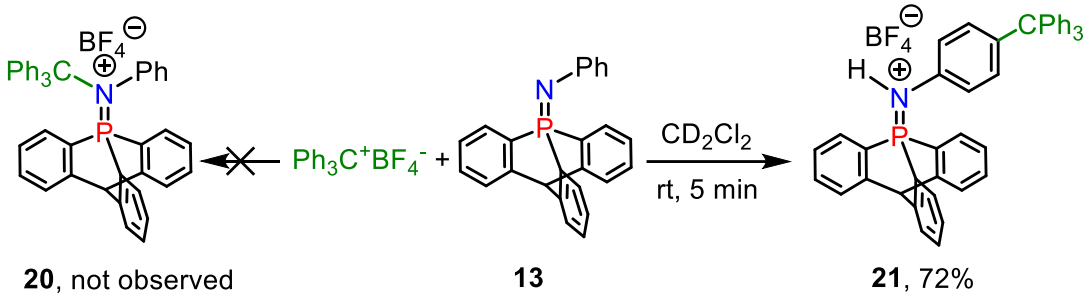
^{13}C NMR (126 MHz, Methylene Chloride-d_2) δ 148.16 (d, J = 7.1 Hz), 144.13 (d, J = 6.4 Hz), 133.52 (d, J = 94.0 Hz), 130.85 (d, J = 1.6 Hz), 129.28 (d, J = 5.0 Hz), 127.35, 126.75 (d, J = 11.6 Hz), 126.41 (d, J = 8.8 Hz), 123.74, 122.69, 54.68 (d, J = 18.5 Hz), 29.44, 24.18.

^{31}P NMR (162 MHz, Methylene Chloride-d_2) δ 26.23, -27.29.

^{11}B NMR (128 MHz, Methylene Chloride-d_2) δ 57.24, -1.60.

^{19}F NMR (376 MHz, Methylene Chloride-d_2) δ -128.06, -133.98 (dd, J = 23.6, 7.6 Hz), -143.80, -157.42 (t, J = 20.2 Hz), -159.52 (t, J = 20.0 Hz), -160.91, -163.60 – -164.69 (m), -165.60 (t, J = 18.8 Hz).

Further investigation of the FLP of **13** with the tritylium ion and subsequent S_EAr reactions the para position of N-Ph of **13** to yield compound **21** (X-ray in Figure S2).



20, not observed **13** **21**, 72%

Compound **21** was prepared by the procedure described below. An NMR tube was charged with tritylium tetrafluoroborate (10.0 mg, 3.05 × 10^{-2} mmol), 9-phospatriptycene imine **13** (10.2 mg, 2.8 × 10^{-2} mmol), and 0.6 mL of CD_2Cl_2 inside a glove box. After measurements of the NMR spectra, the solvent was slowly evaporated inside glove box to get the crystals suitable for X-ray analysis (14.0 mg, 2.02× 10^{-2} mmol, 72%).

^{1}H NMR (500 MHz, Methylene Chloride-d_2) δ 8.70 (d, J = 2.6 Hz, 1H), 7.94 (ddd, J = 13.4, 7.3, 2.5 Hz, 3H), 7.76 (dq, J = 7.8, 3.2, 2.2 Hz, 3H), 7.51 – 7.43 (m, 4H), 7.39 (dd, J = 8.8, 2.3 Hz, 2H), 7.31 (d, J = 8.8 Hz, 4H), 7.30 – 7.28 (m, 4H), 7.28 – 7.25 (m, 8H), 7.25 – 7.21 (m, 5H), 5.86 (s, 1H).

^{13}C NMR (126 MHz, Methylene Chloride-d_2) δ 146.96 (d, J = 7.6 Hz), 146.55, 132.67 (d, J = 29.3 Hz), 131.03, 130.16, 129.47 (d, J = 5.4 Hz), 127.90 (d, J = 7.1 Hz), 127.68, 127.19 (dd, J = 13.1, 3.2 Hz), 126.88 (dd, J = 9.9, 4.0 Hz), 126.15, 120.00 (d, J = 8.3 Hz), 119.41 (d, J = 7.7 Hz), 64.62, 54.67 (d, J = 21.8 Hz).

^{31}P NMR (202 MHz, Methylene Chloride-d_2) δ 9.41.

^{11}B NMR (160 MHz, Methylene Chloride-d_2) δ -1.76.

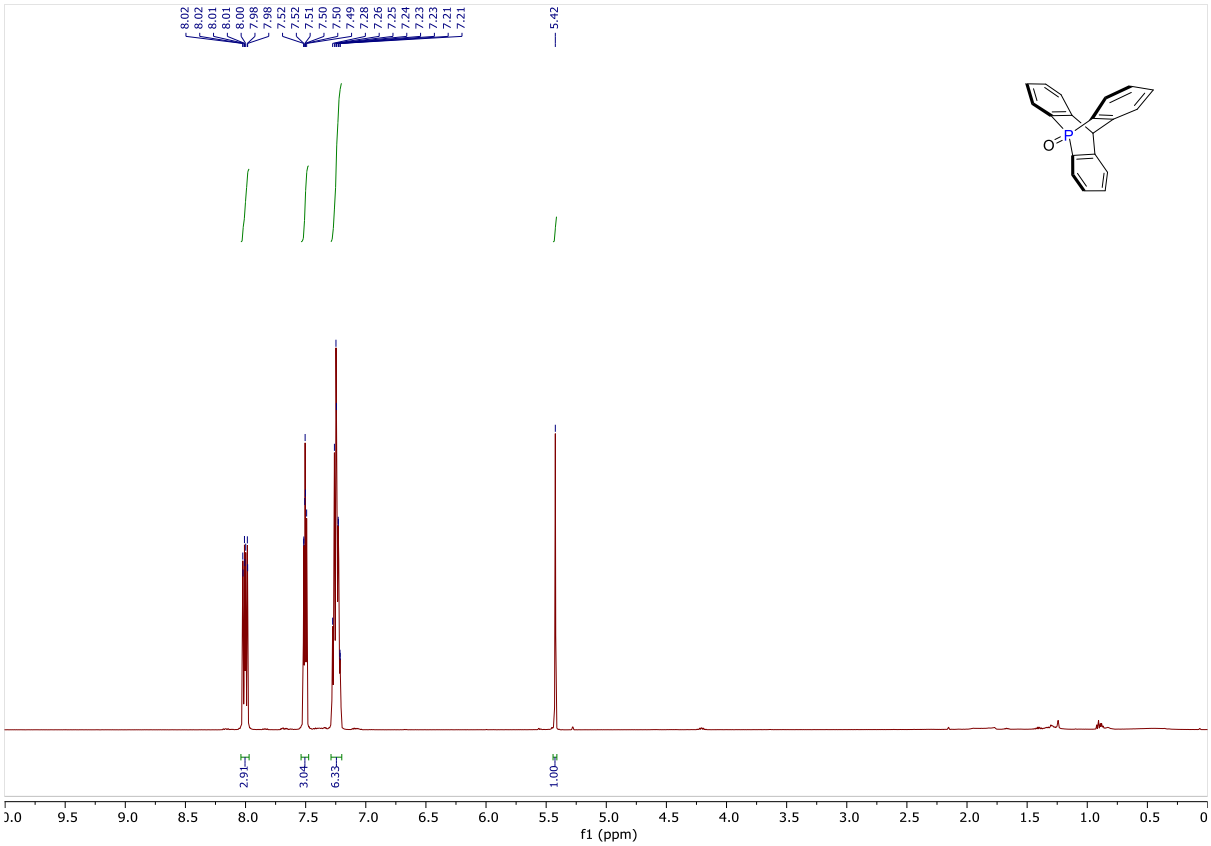
^{19}F NMR (471 MHz, Methylene Chloride-d_2) δ -148.66.

IR (neat, ATR): $\tilde{\nu}$ / cm^{-1} = 3220, 1609, 1588, 1511, 1493, 1444, 1271, 1228, 1110, 1067, 989, 855, 827, 769, 759, 705, 630, 610, 549, 522.

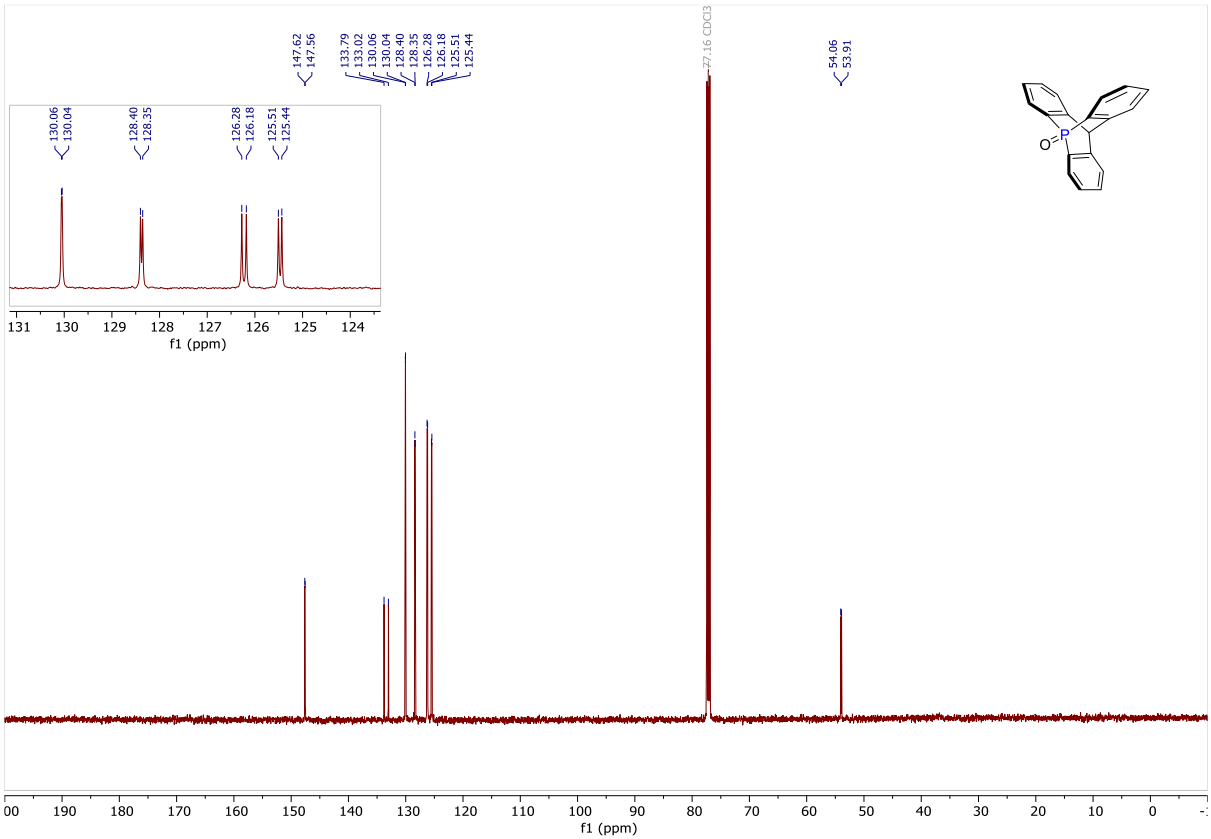
HRMS (ESI$^+$): Calcd. for $C_{44}H_{33}NP^+$ $[M]^+$: 606.2346, found: 606.2395.

M.p.: 309-311 °C (dec)

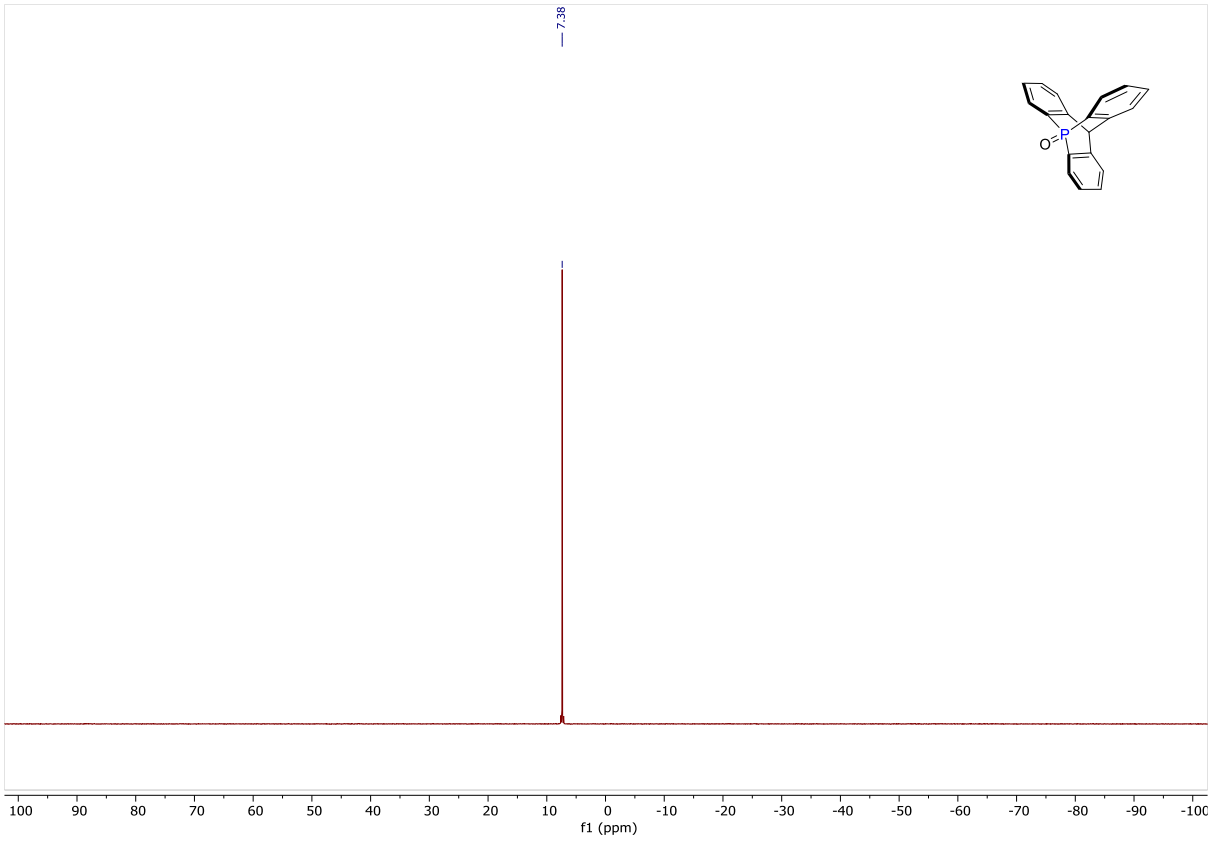
4. Copies of all NMR spectra



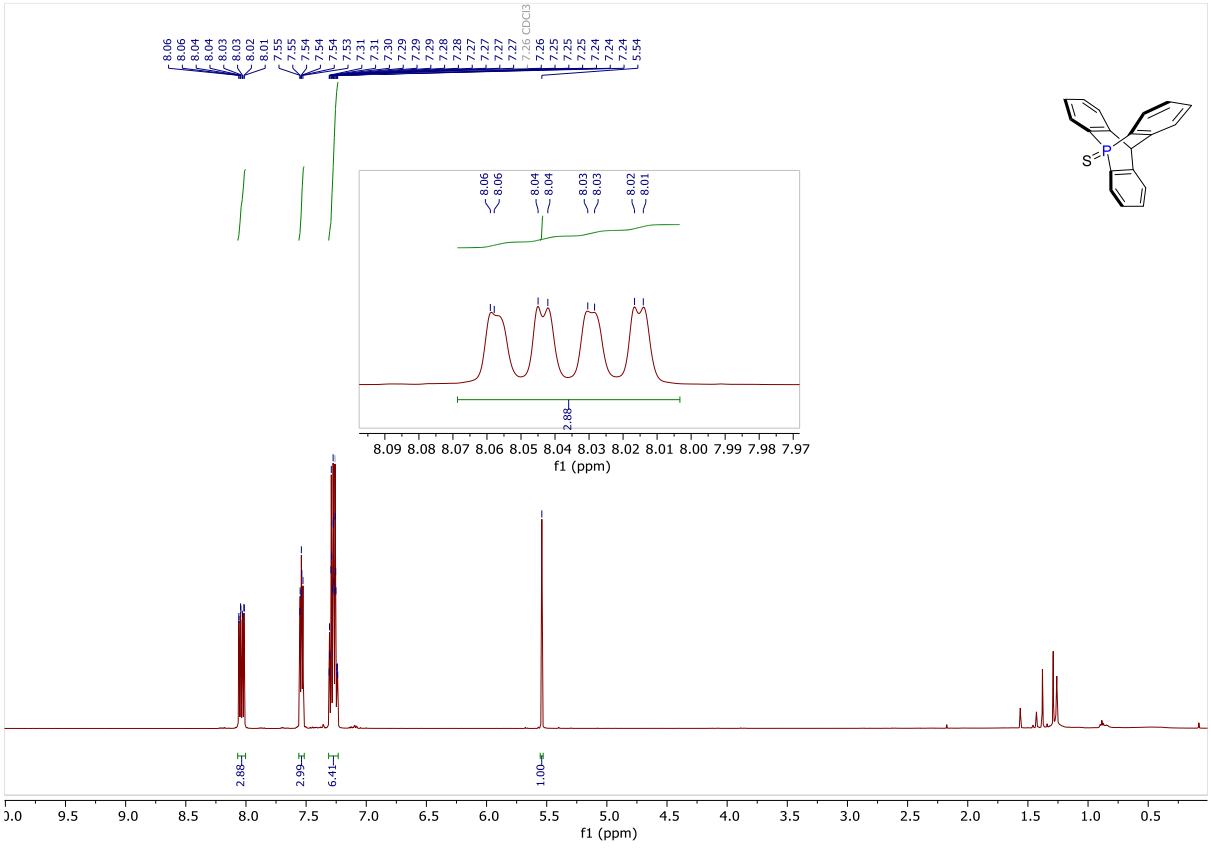
^{1}H NMR (500 MHz, 25 °C, $CDCl_3$) of **6**



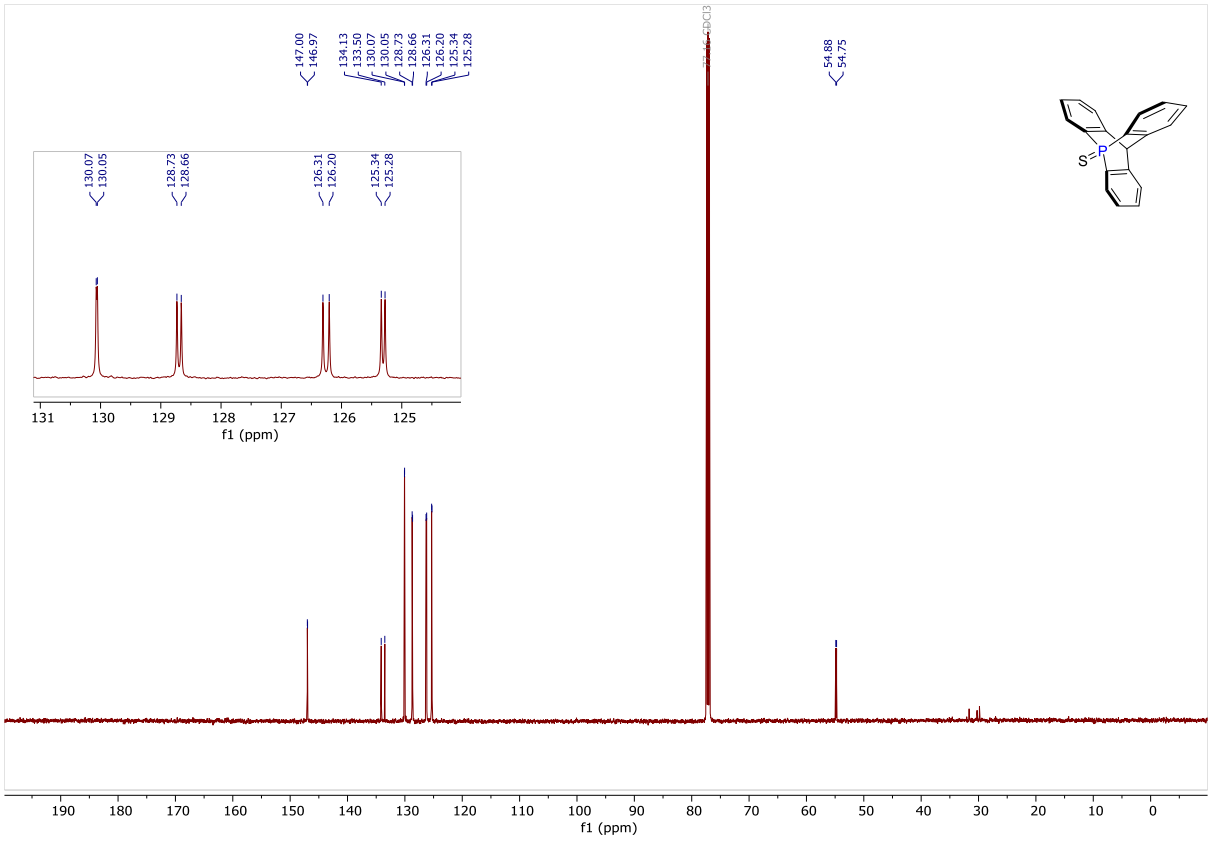
^{13}C NMR (126 MHz, 25 °C, $CDCl_3$) of **6**



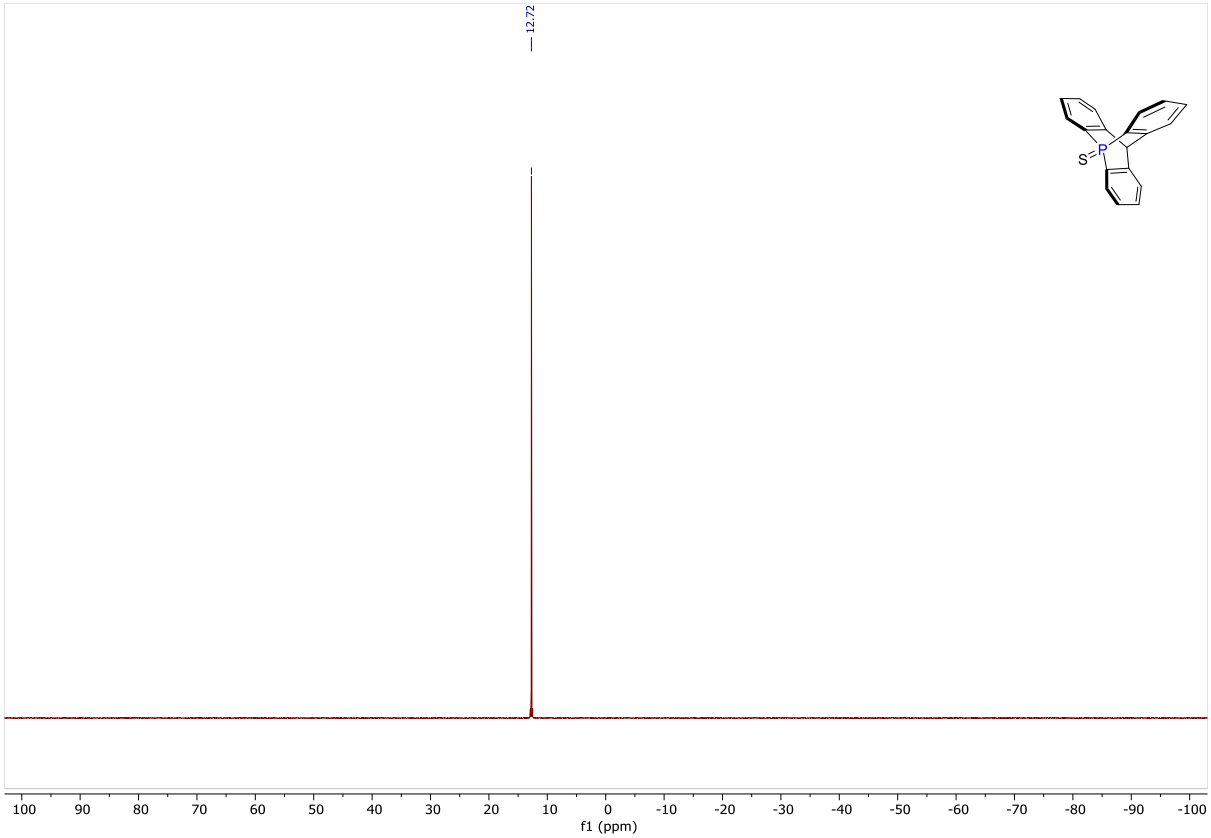
^{31}P NMR (202 MHz, 25 °C, $CDCl_3$) of **6**



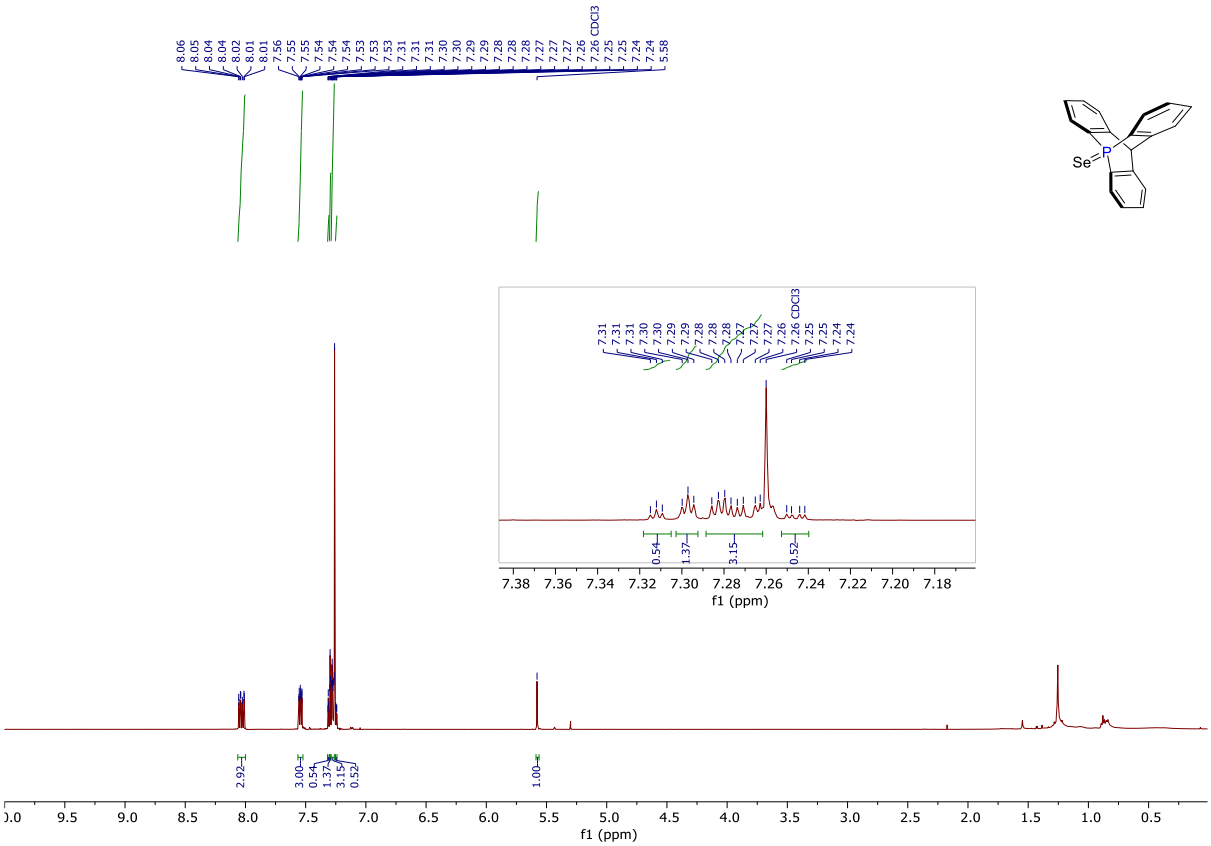
^{1}H NMR (500 MHz, 25 °C, $CDCl_3$) of **7**



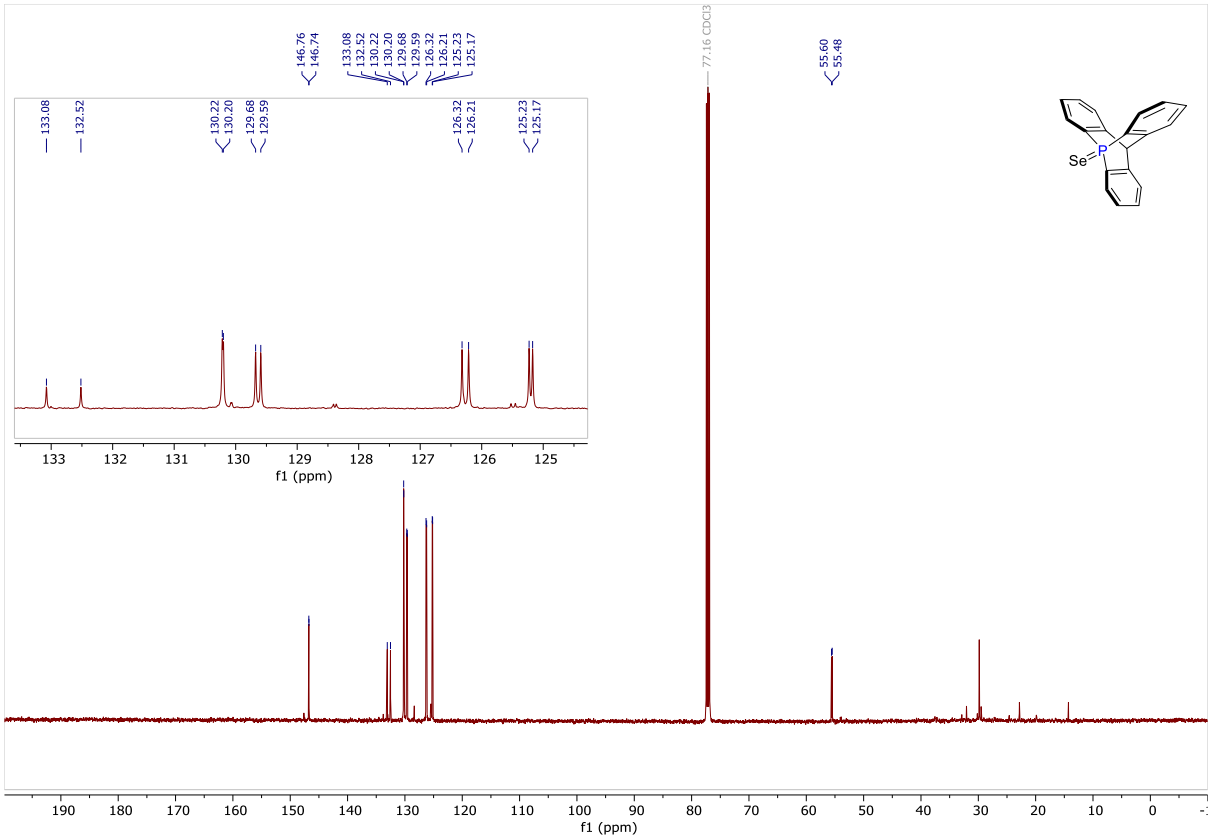
^{13}C NMR (126 MHz, 25 °C, $CDCl_3$) of **7**



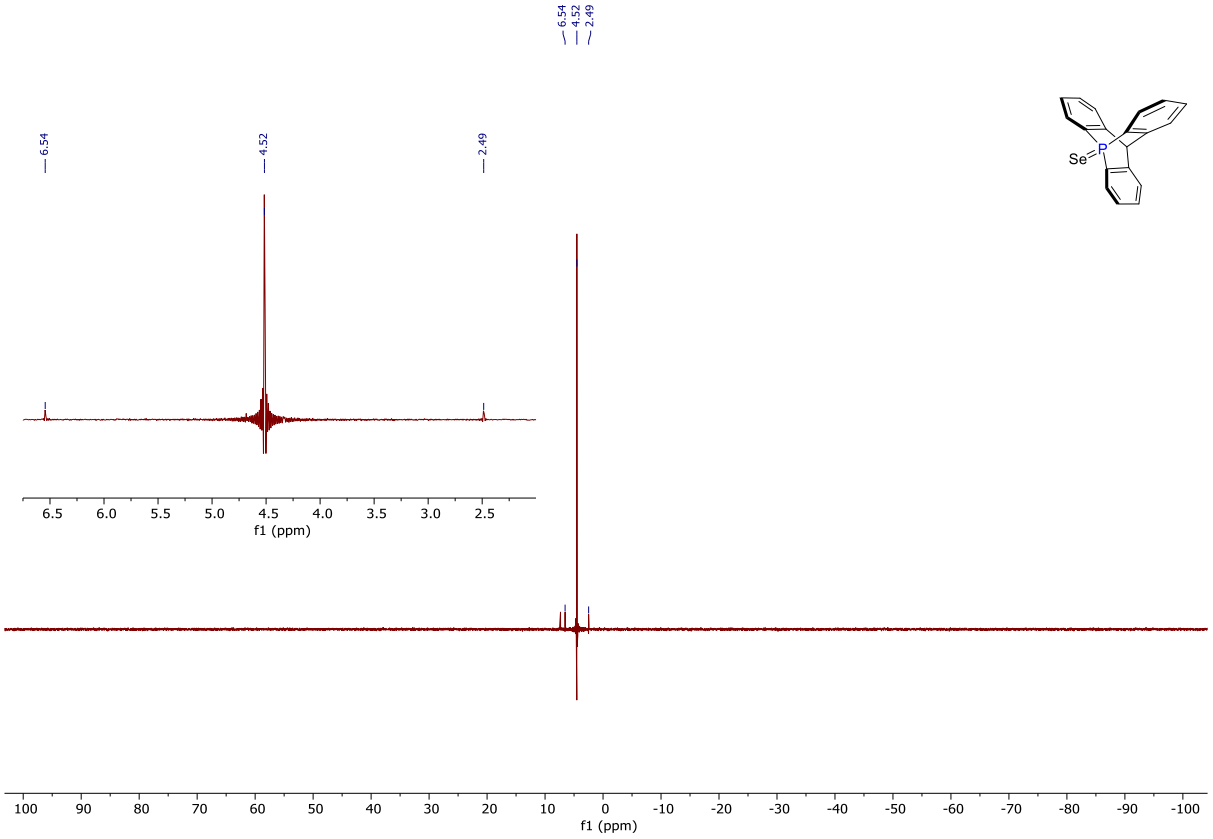
^{31}P NMR (202 MHz, 25 °C, $CDCl_3$) of **7**



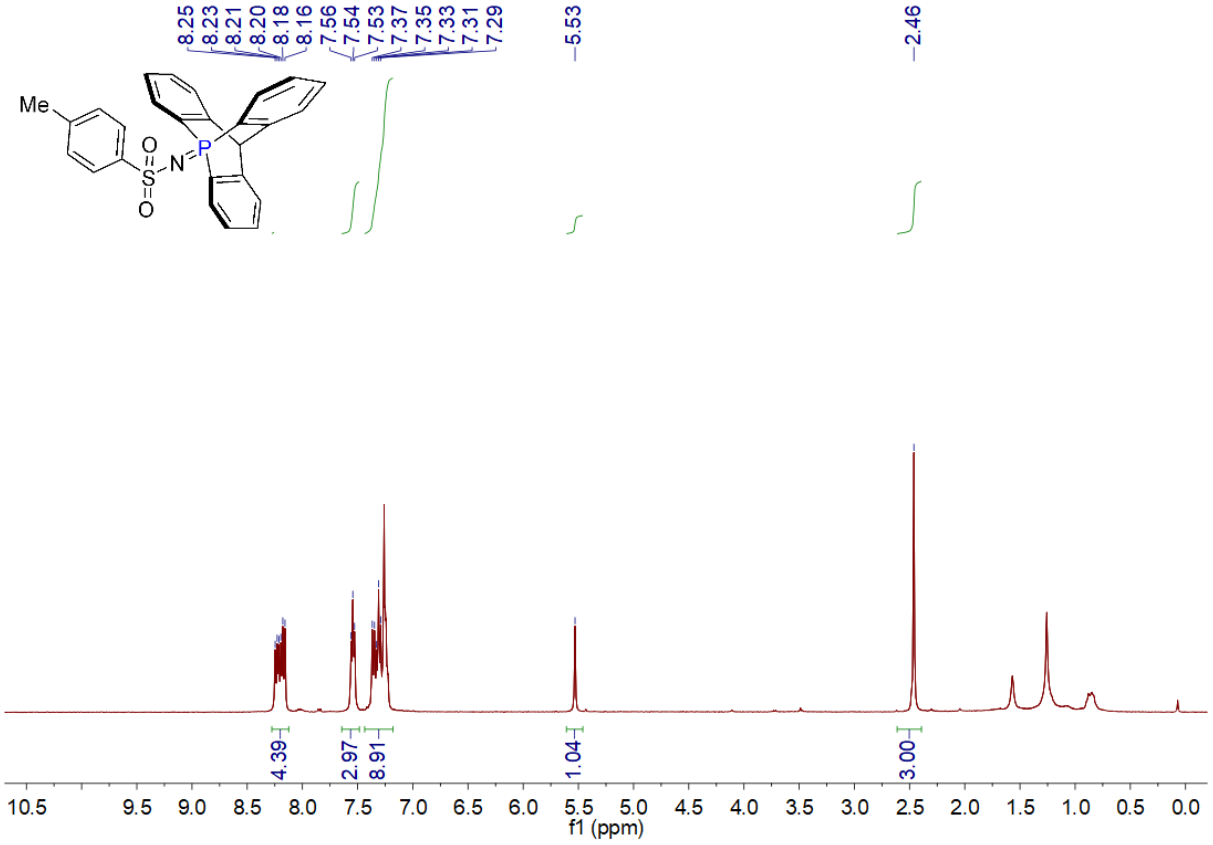
^{1}H NMR (500 MHz, 25 °C, $CDCl_3$) of **8**



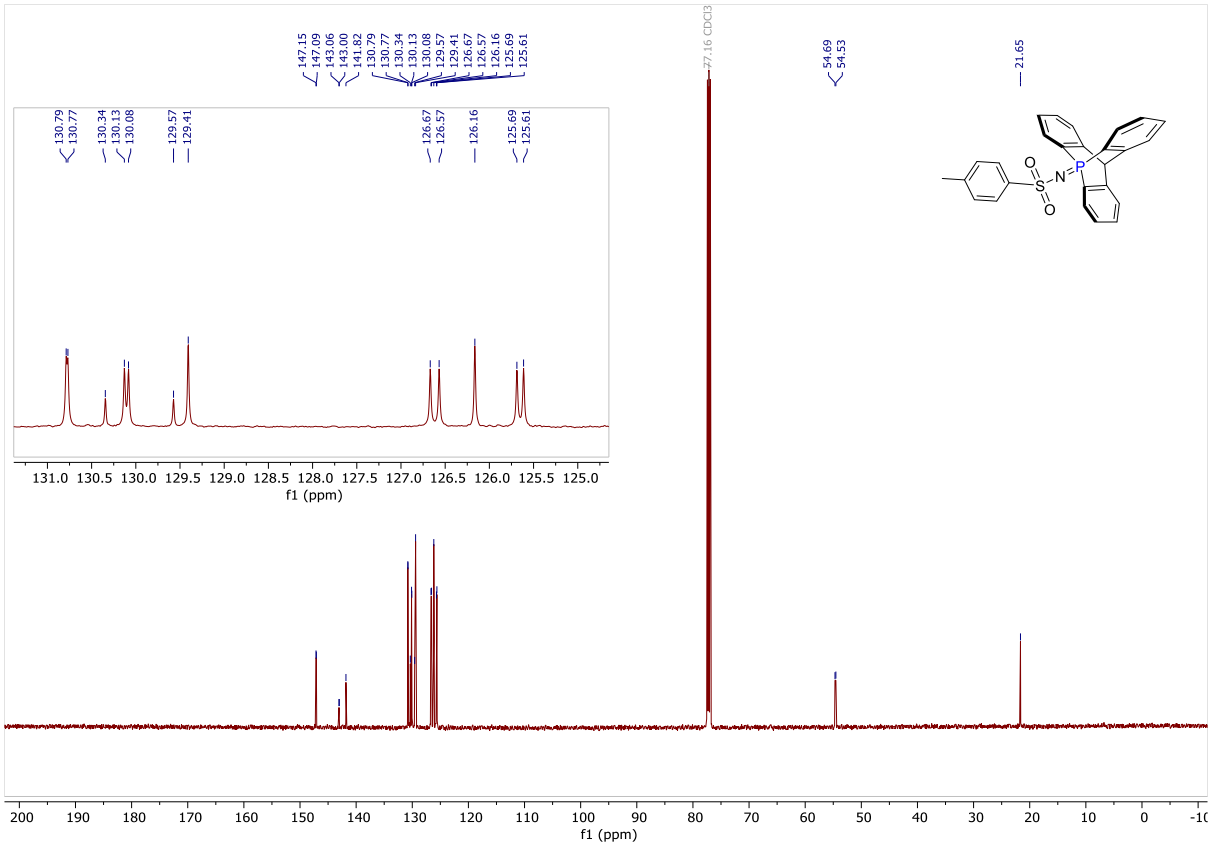
^{13}C NMR (126 MHz, 25 °C, $CDCl_3$) of **8**



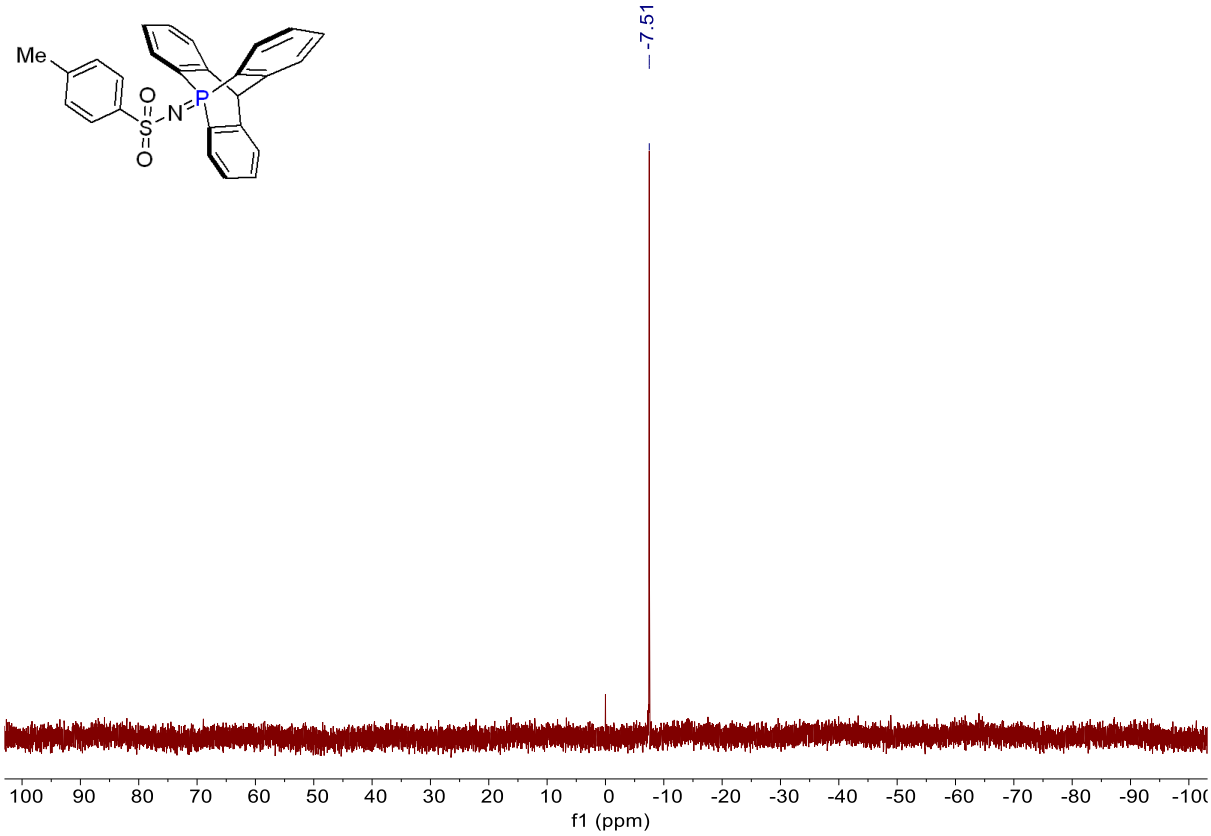
^{31}P NMR (202 MHz, 25 °C, $CDCl_3$) of **8**



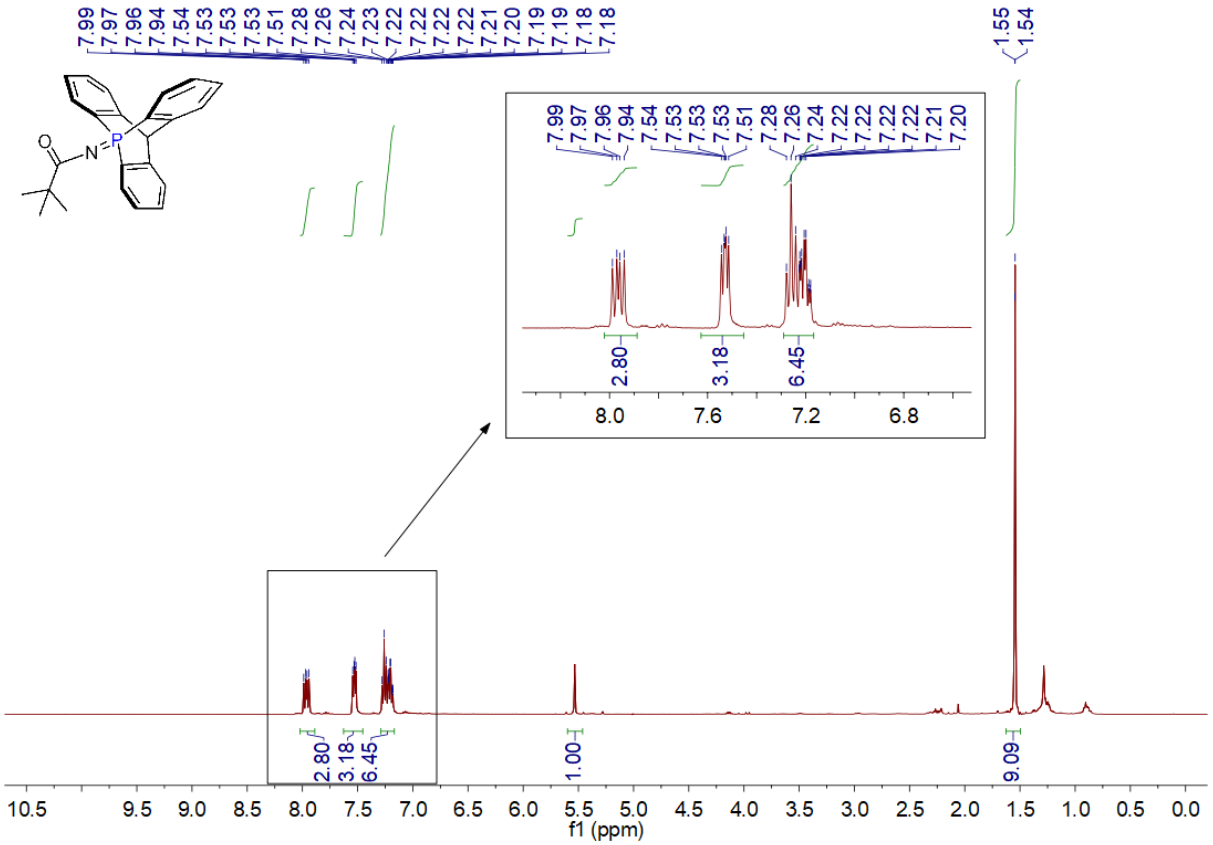
^{1}H NMR (400 MHz, 25 °C, $CDCl_3$) of **9**



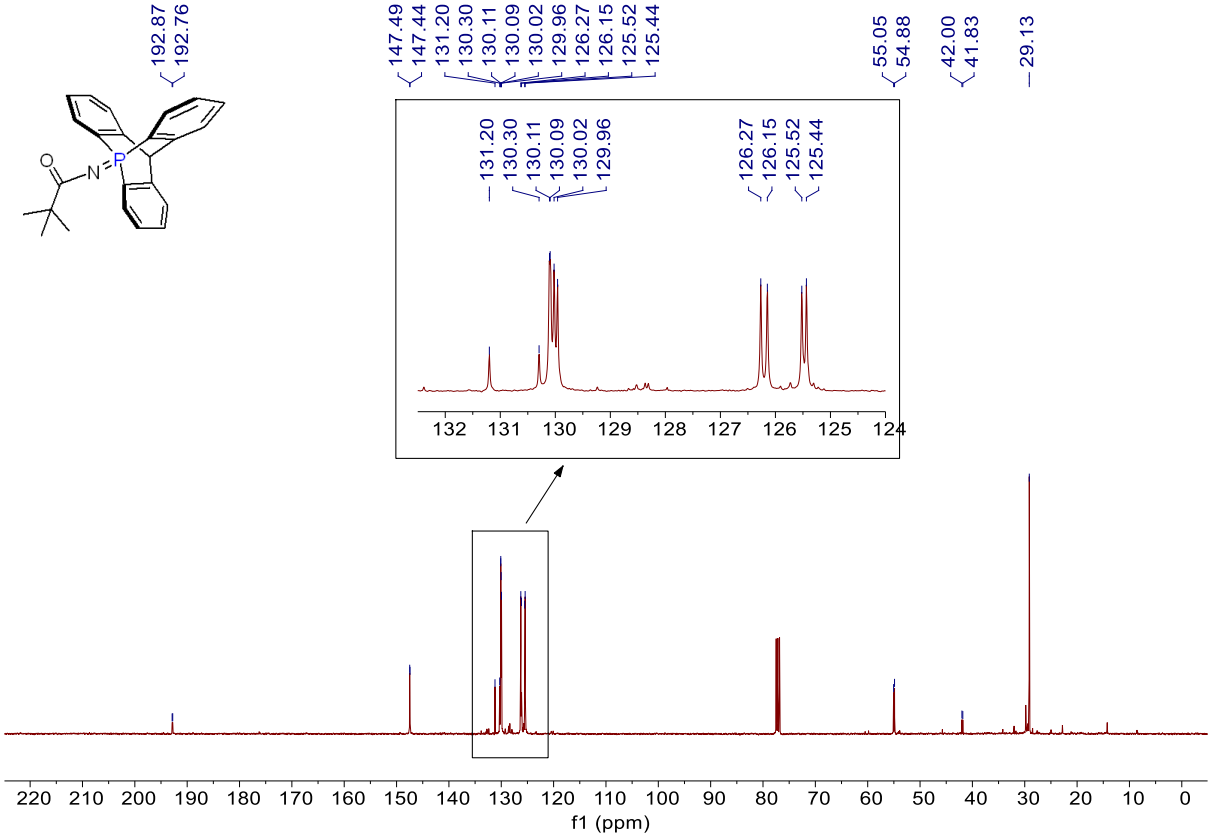
^{13}C NMR (126 MHz, 25 °C, $CDCl_3$) of **9**



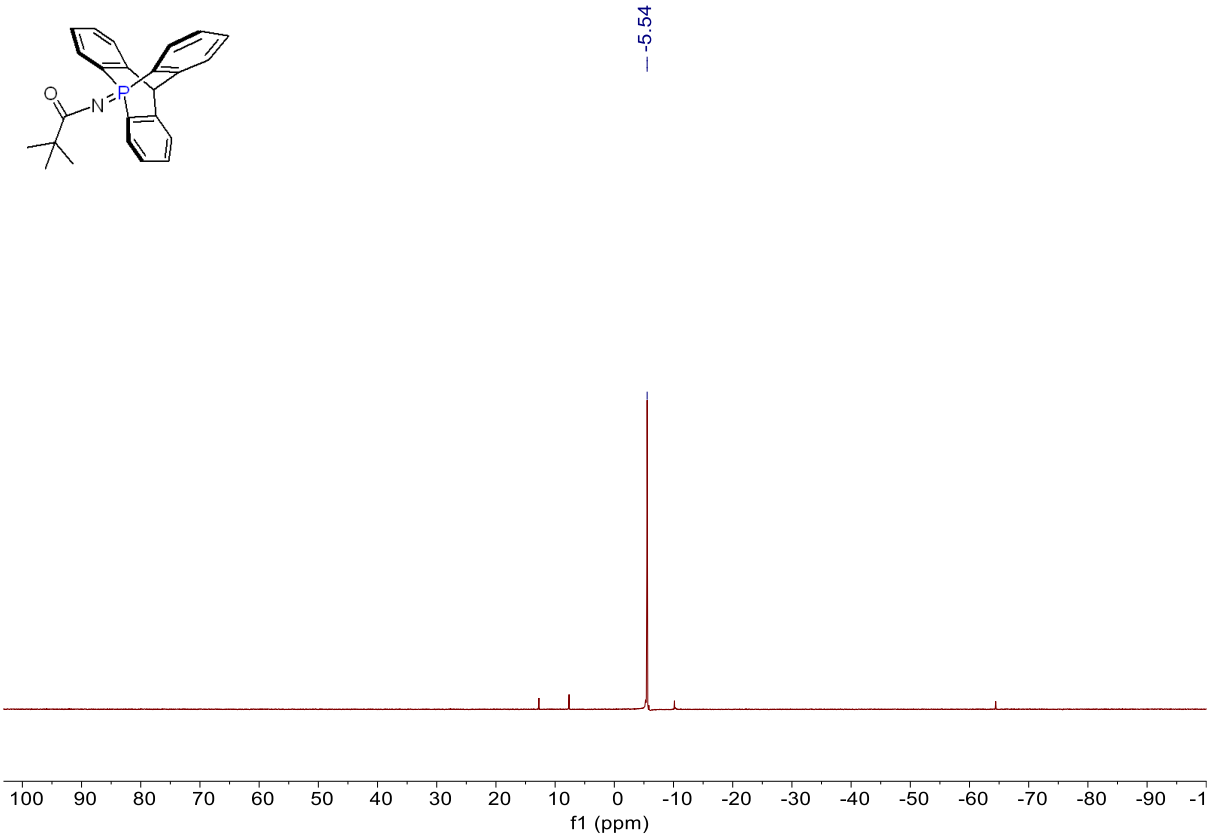
^{31}P NMR (161 MHz, 25 °C, $CDCl_3$) of **9**



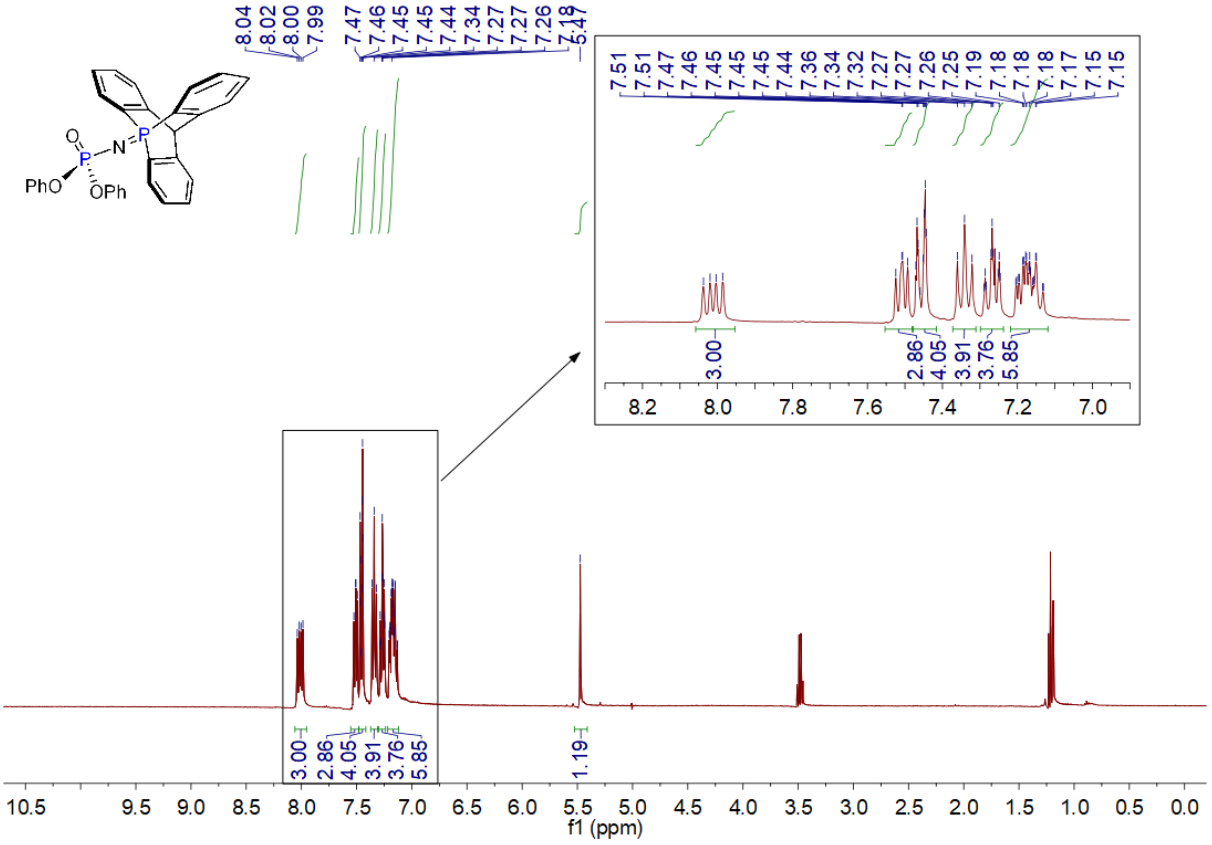
^{1}H NMR (400 MHz, 25 °C, $CDCl_3$) of **10**



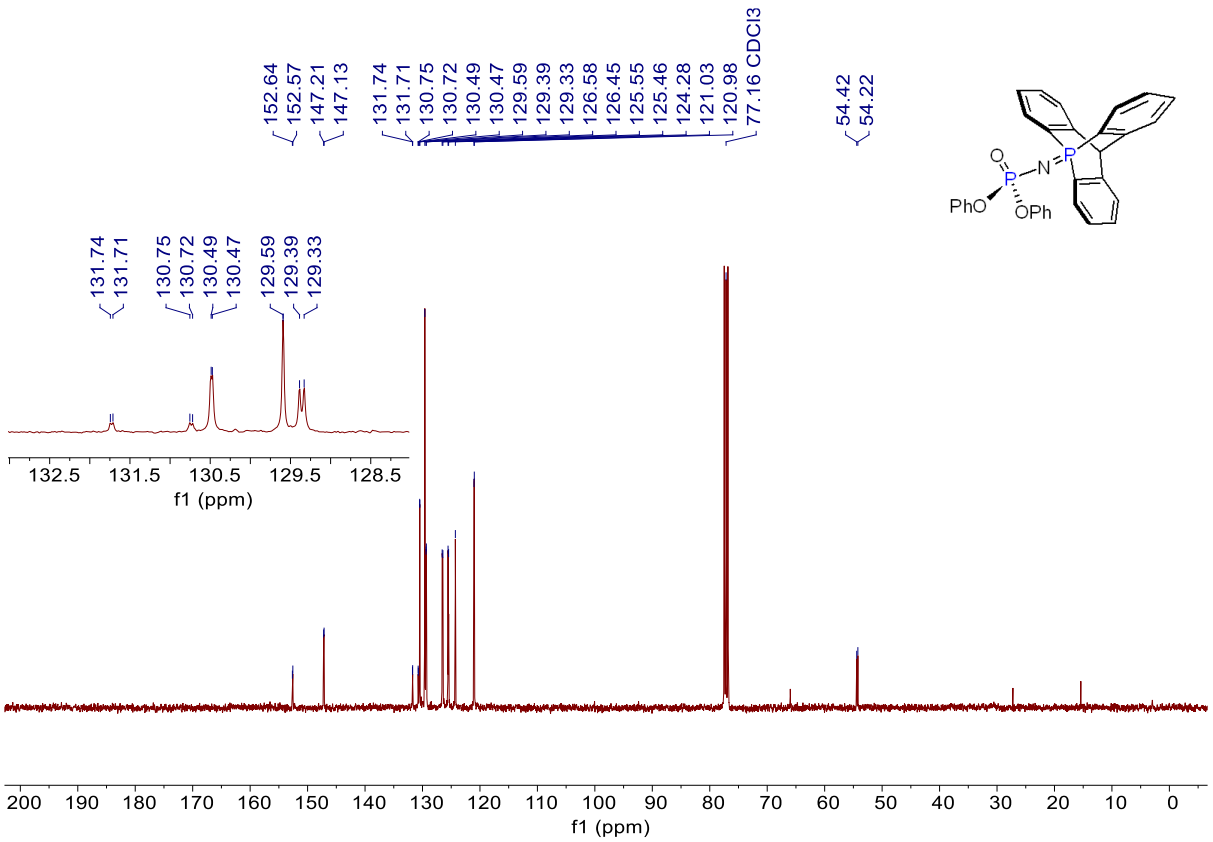
^{13}C NMR (100 MHz, 25 °C, $CDCl_3$) of **10**



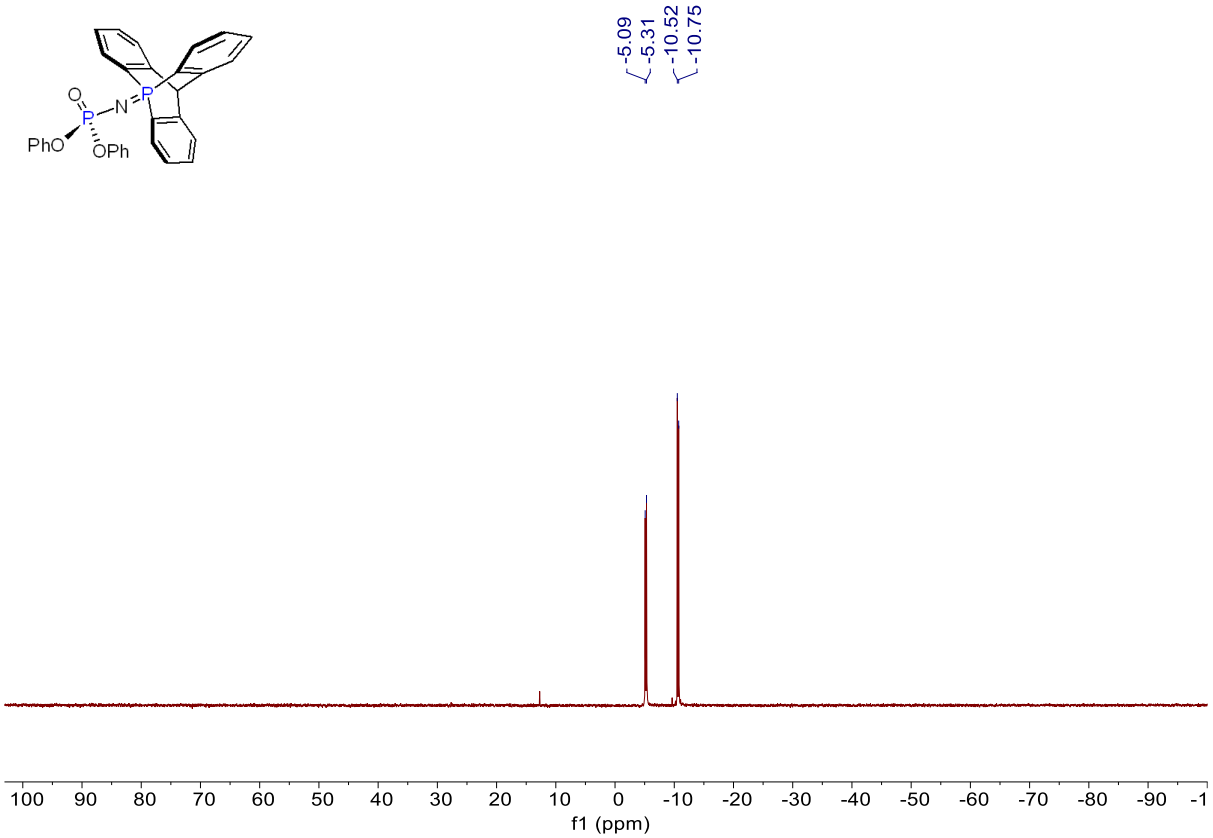
^{31}P NMR (161 MHz, 25 °C, $CDCl_3$) of **10**



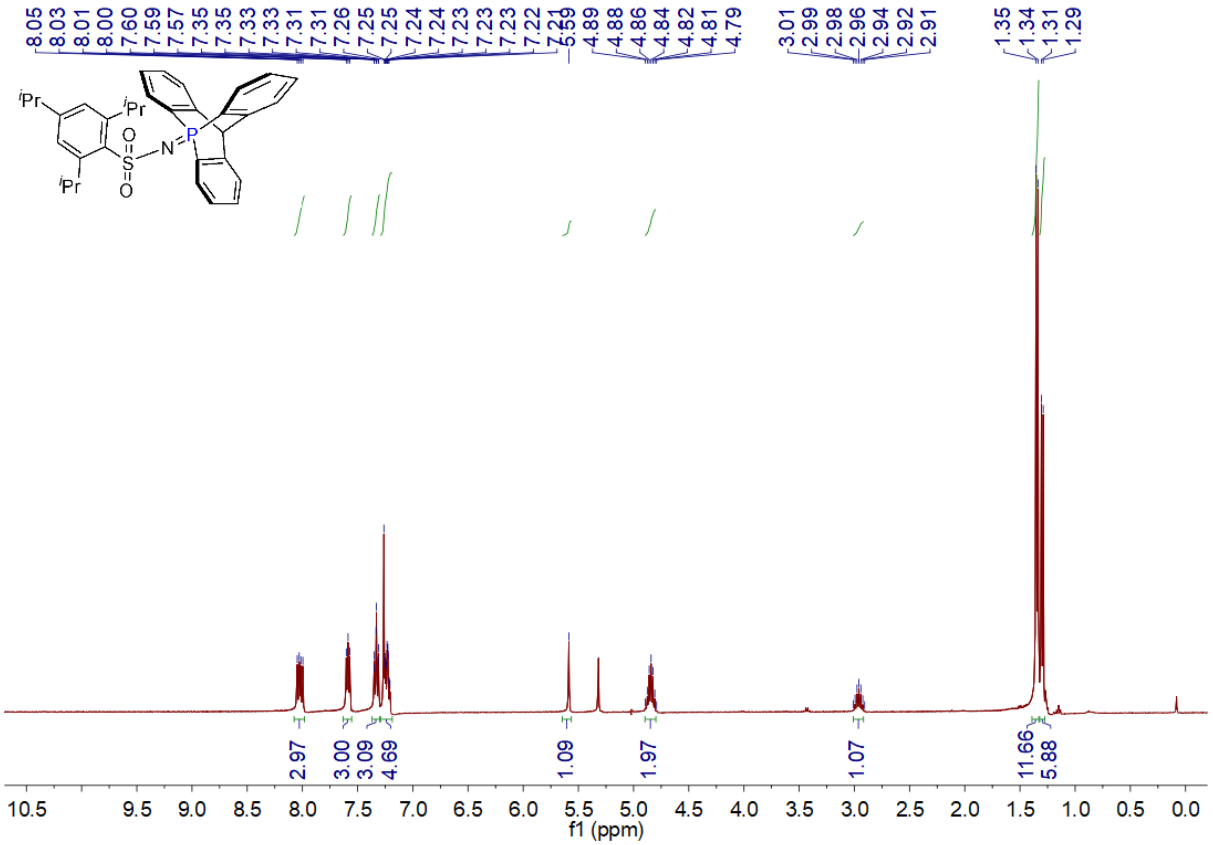
^{1}H NMR (400 MHz, 25 °C, $CDCl_3$) of **11**



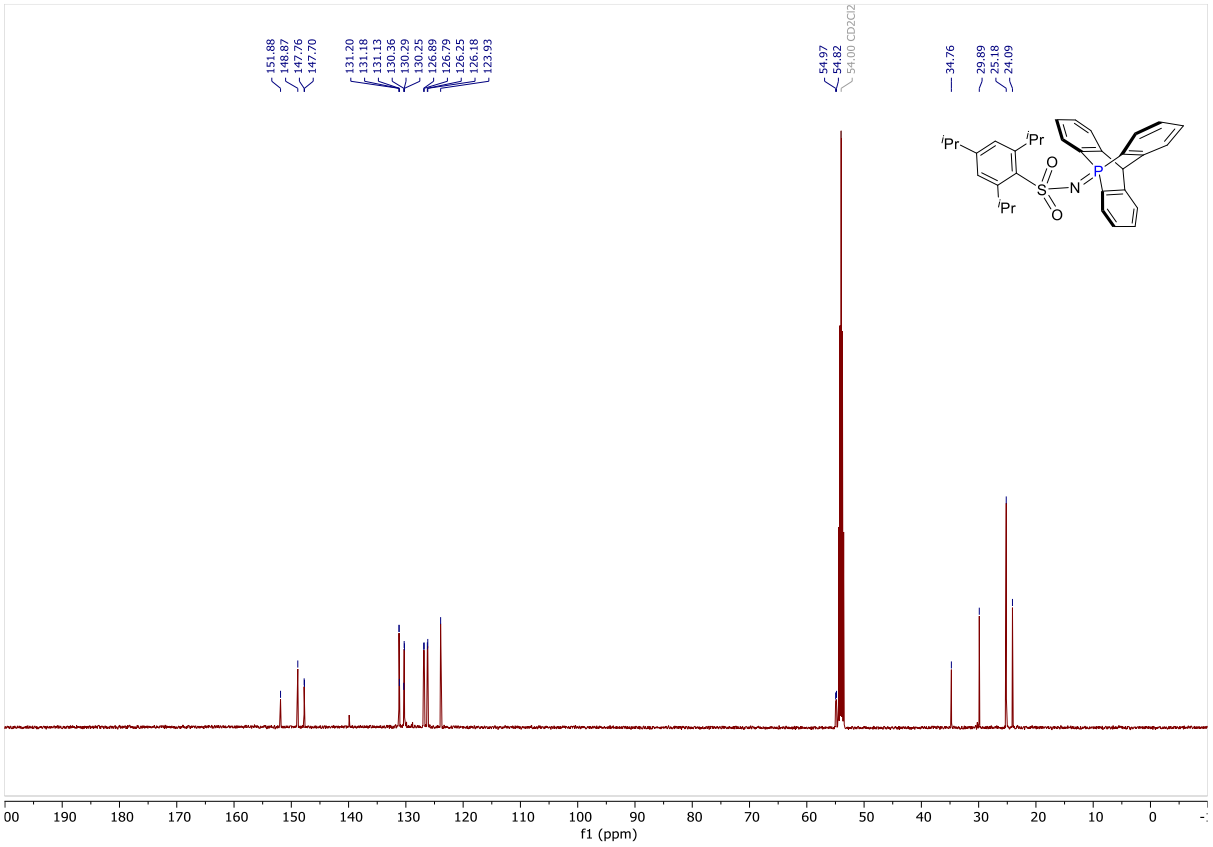
^{13}C NMR (100 MHz, 25 °C, $CDCl_3$) of **11**



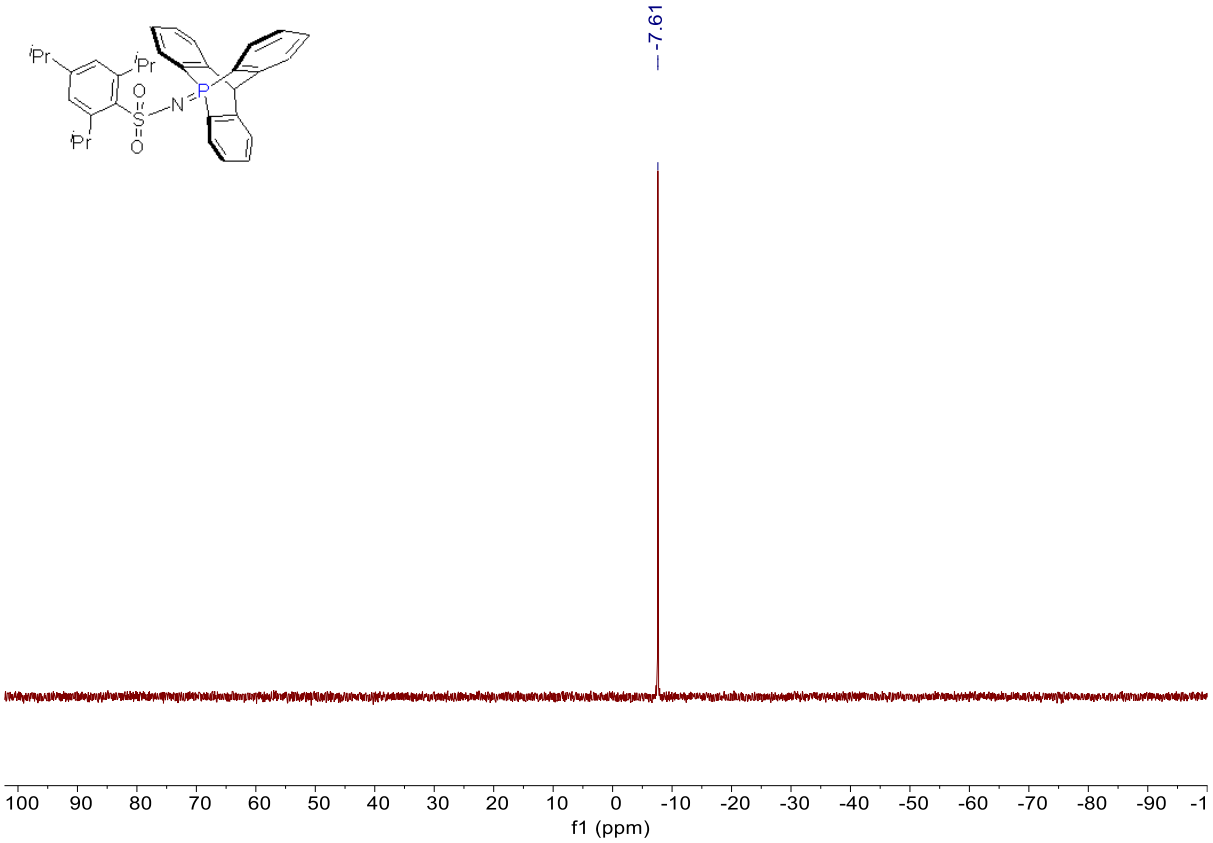
^{31}P NMR (161 MHz, 25 °C, $CDCl_3$) of **11**



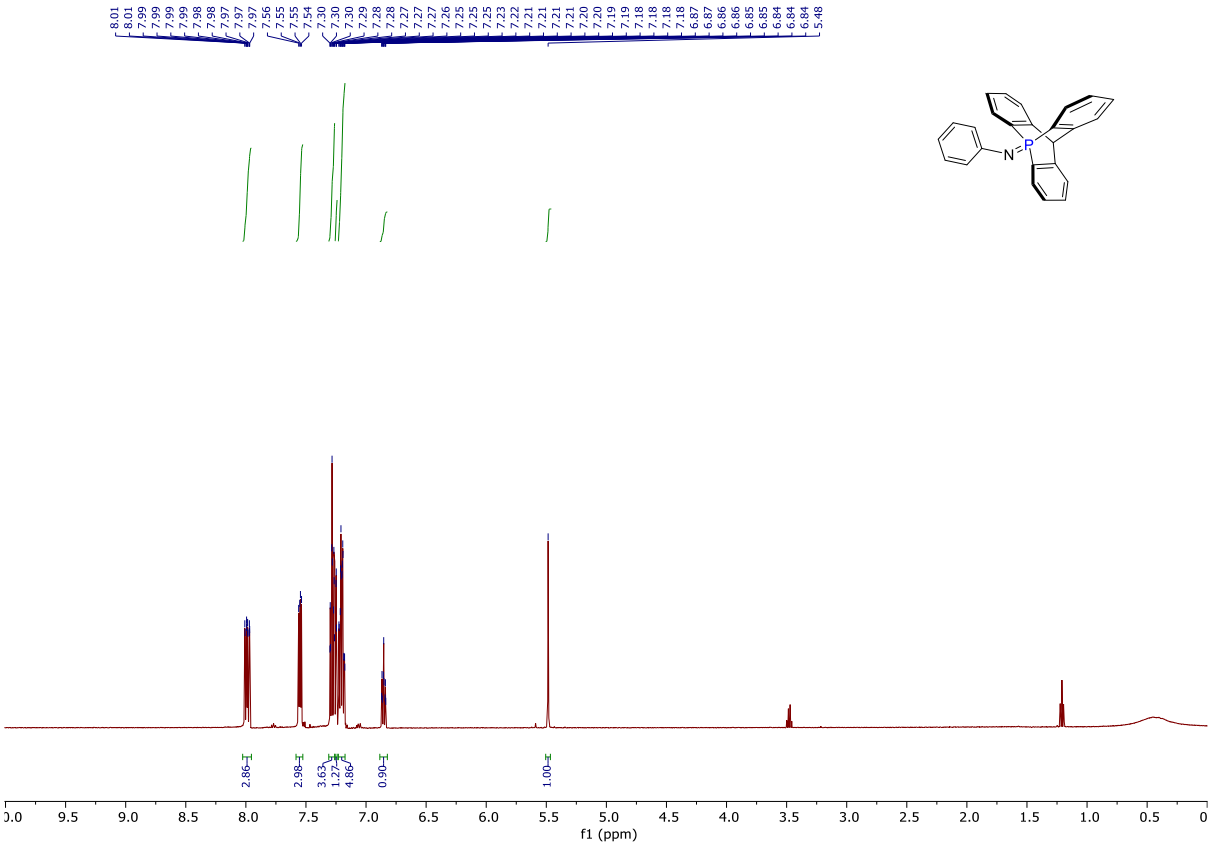
^{1}H NMR (400 MHz, 25 °C, CD_2Cl_2) of **12**



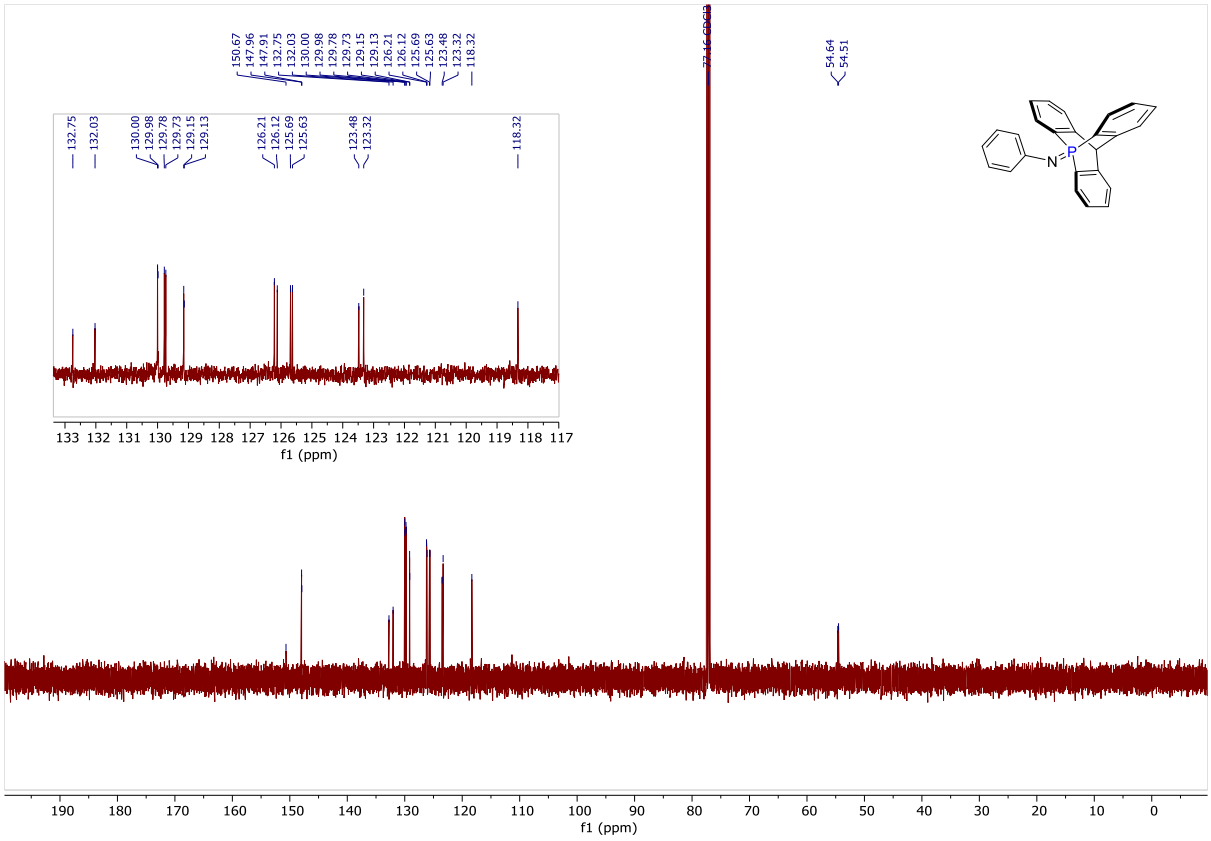
^{13}C NMR (126 MHz, 25 °C, CD_2Cl_2) of **12**



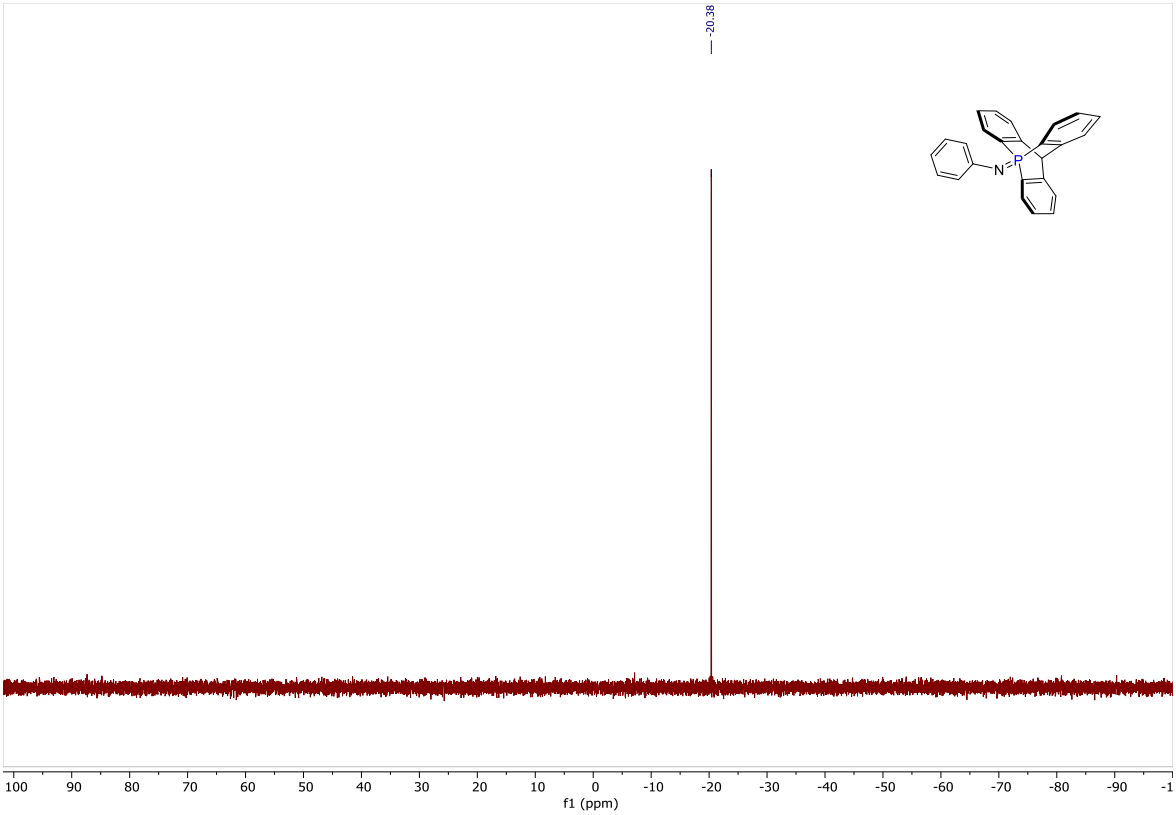
^{31}P NMR (161 MHz, 25 °C, CD_2Cl_2) of **12**



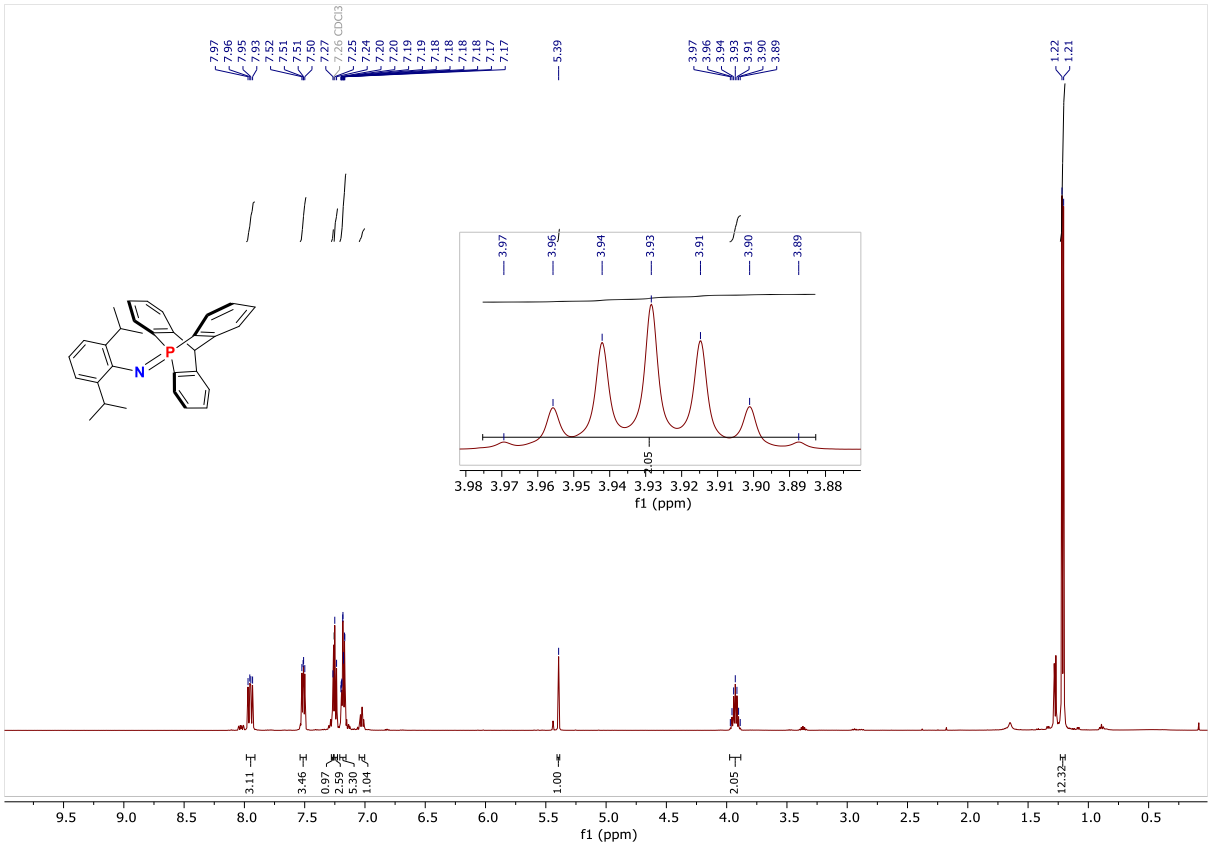
^{1}H NMR (500 MHz, 25 °C, $CDCl_3$) of **13**



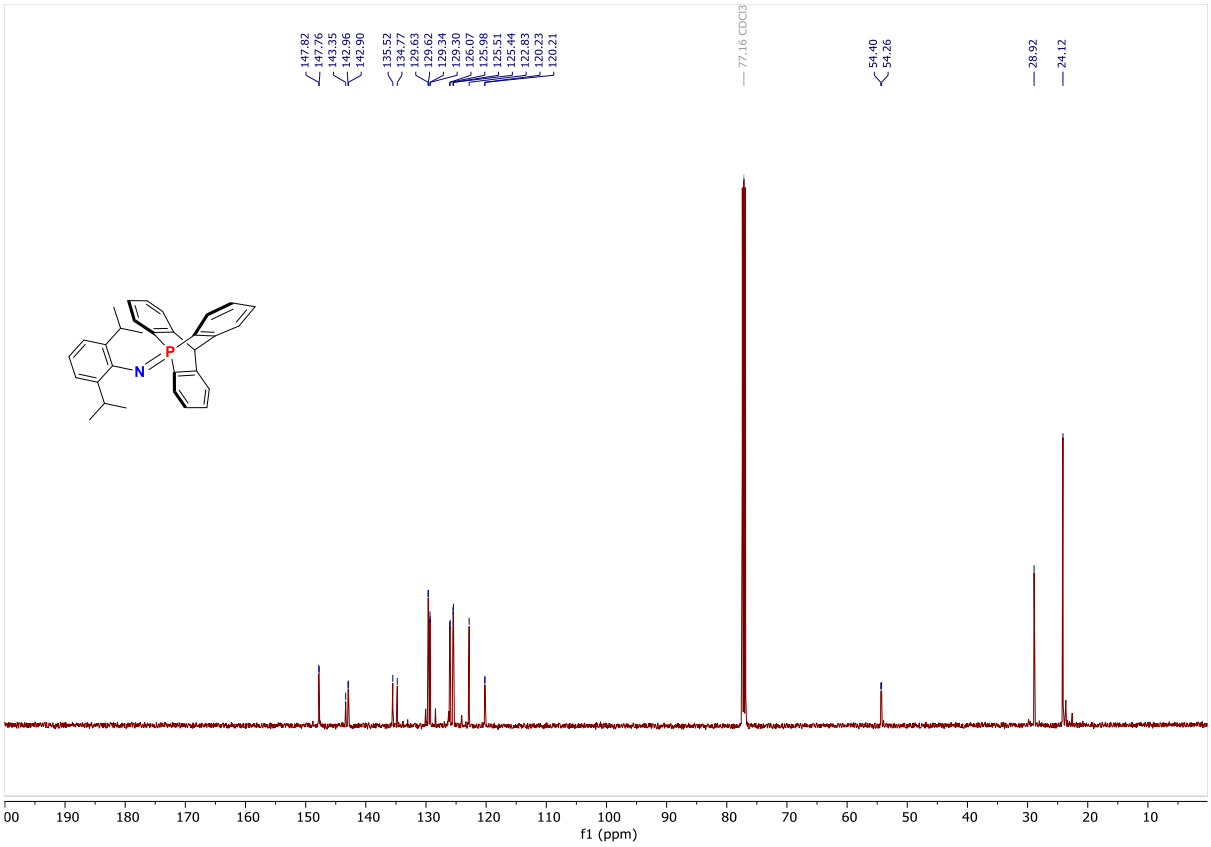
^{13}C NMR (126 MHz, 25 °C, $CDCl_3$) of **13**



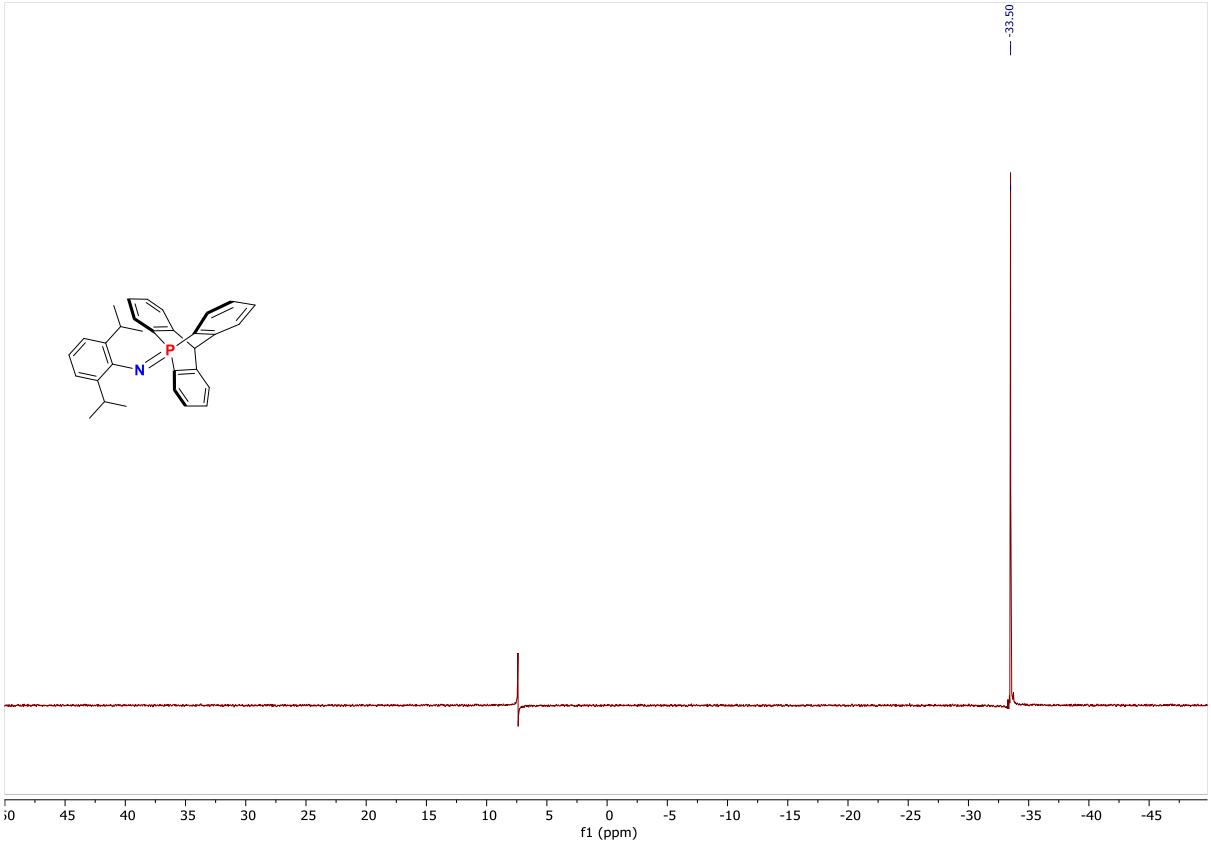
^{31}P NMR (202 MHz, 25 °C, $CDCl_3$) of **13**



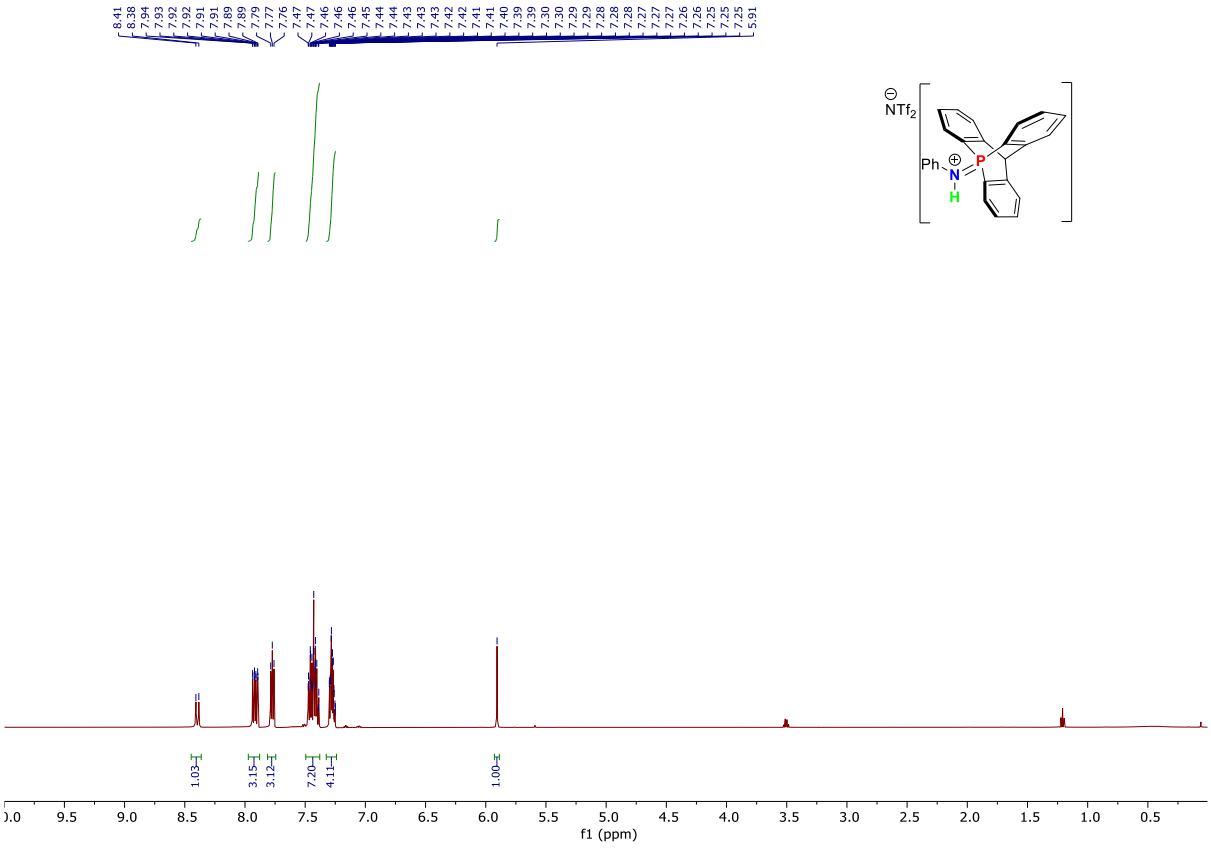
^{1}H NMR (500 MHz, 25 °C, $CDCl_3$) of **14**



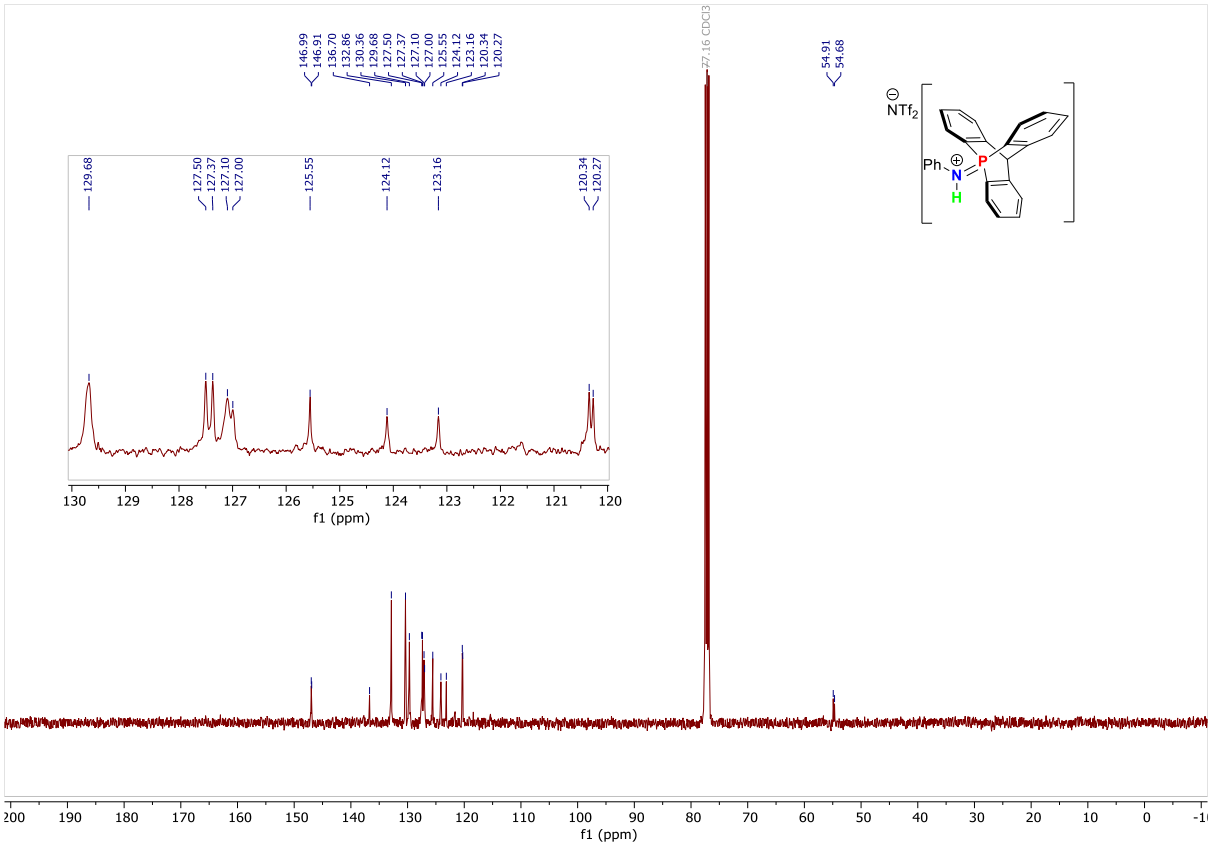
^{13}C NMR (126 MHz, 25 °C, $CDCl_3$) of **14**



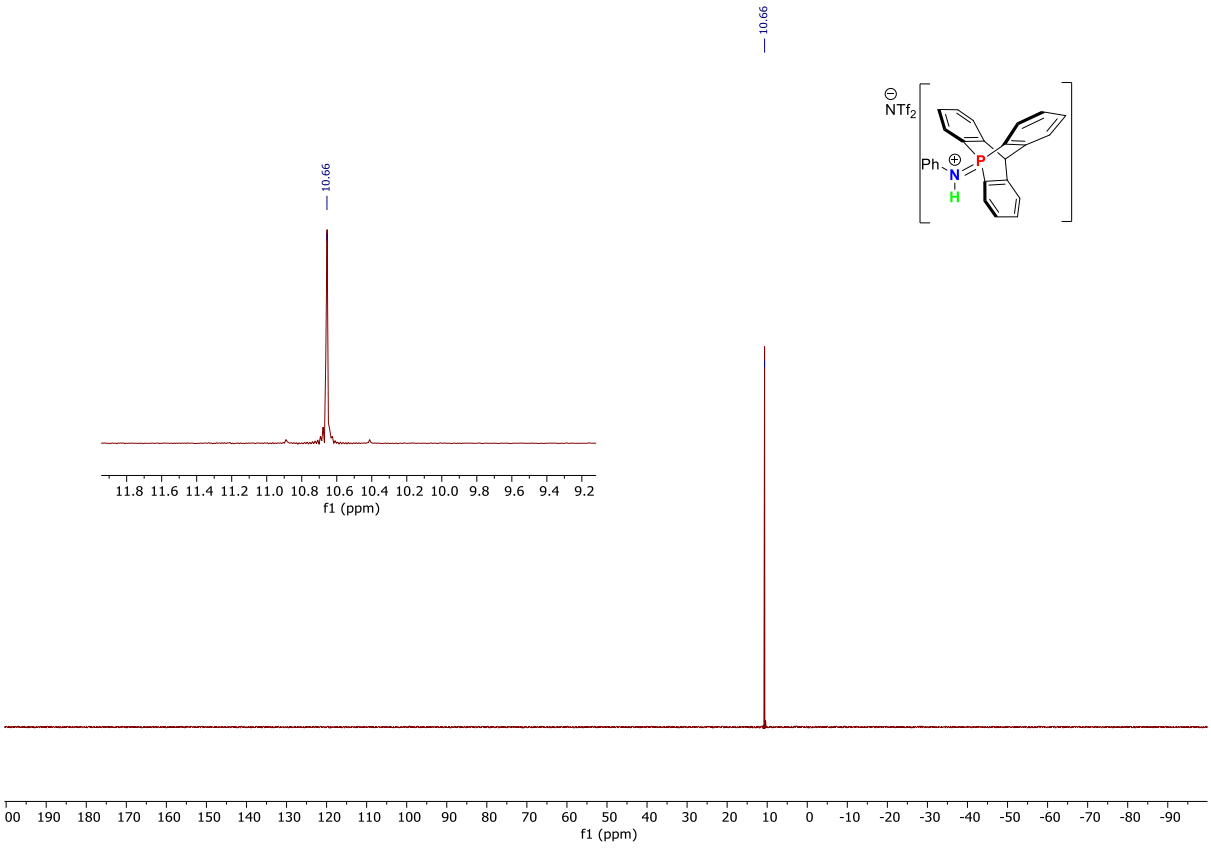
^{31}P NMR (202 MHz, 25 °C, $CDCl_3$) of **14**



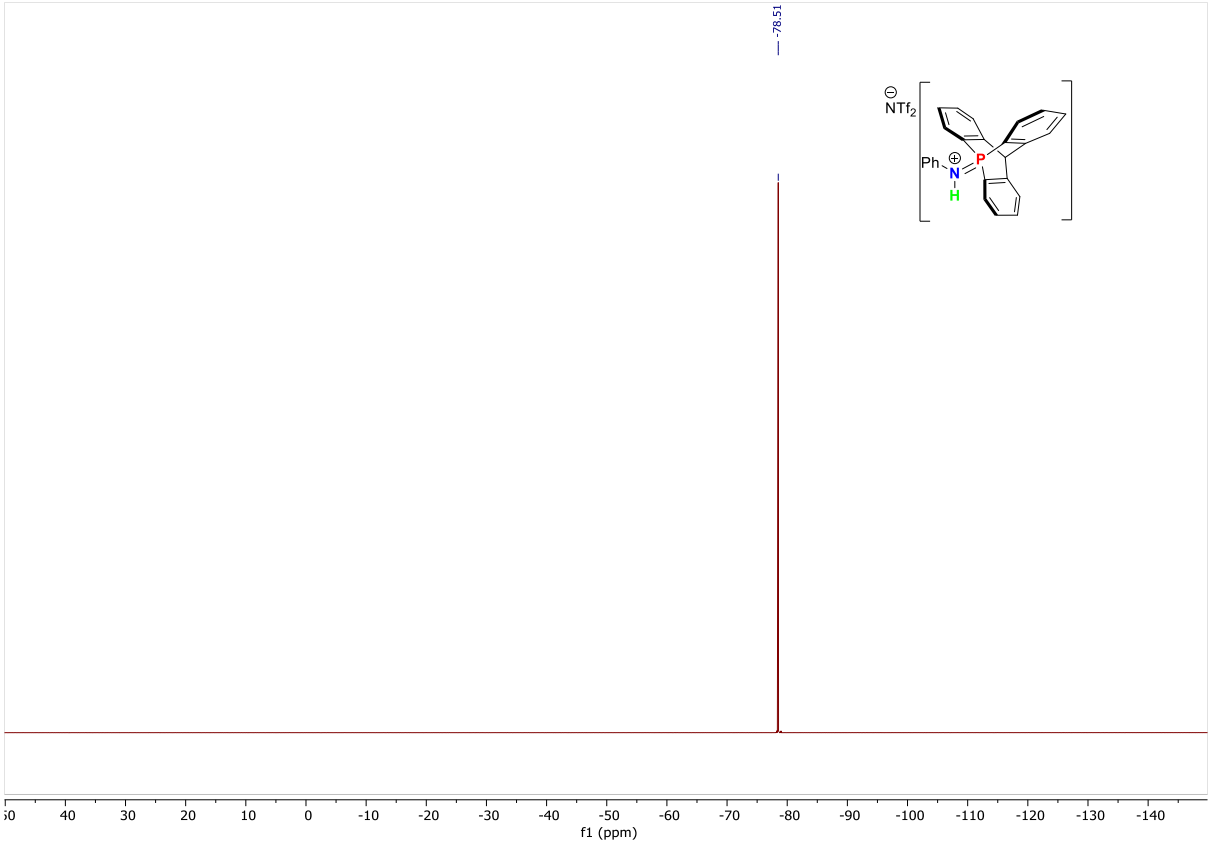
^{1}H NMR (500 MHz, 25 °C, $CDCl_3$) of **15**



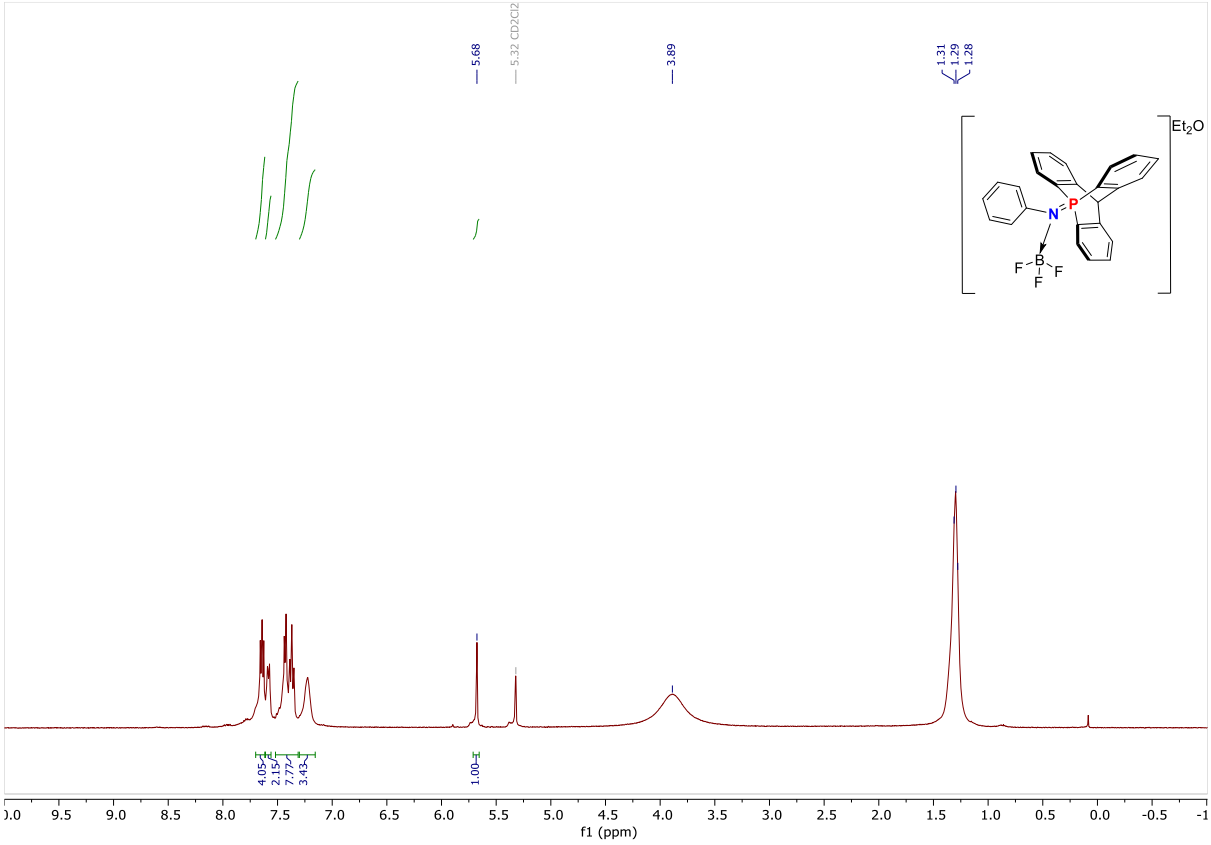
^{13}C NMR (101 MHz, 25 °C, $CDCl_3$) of **15**



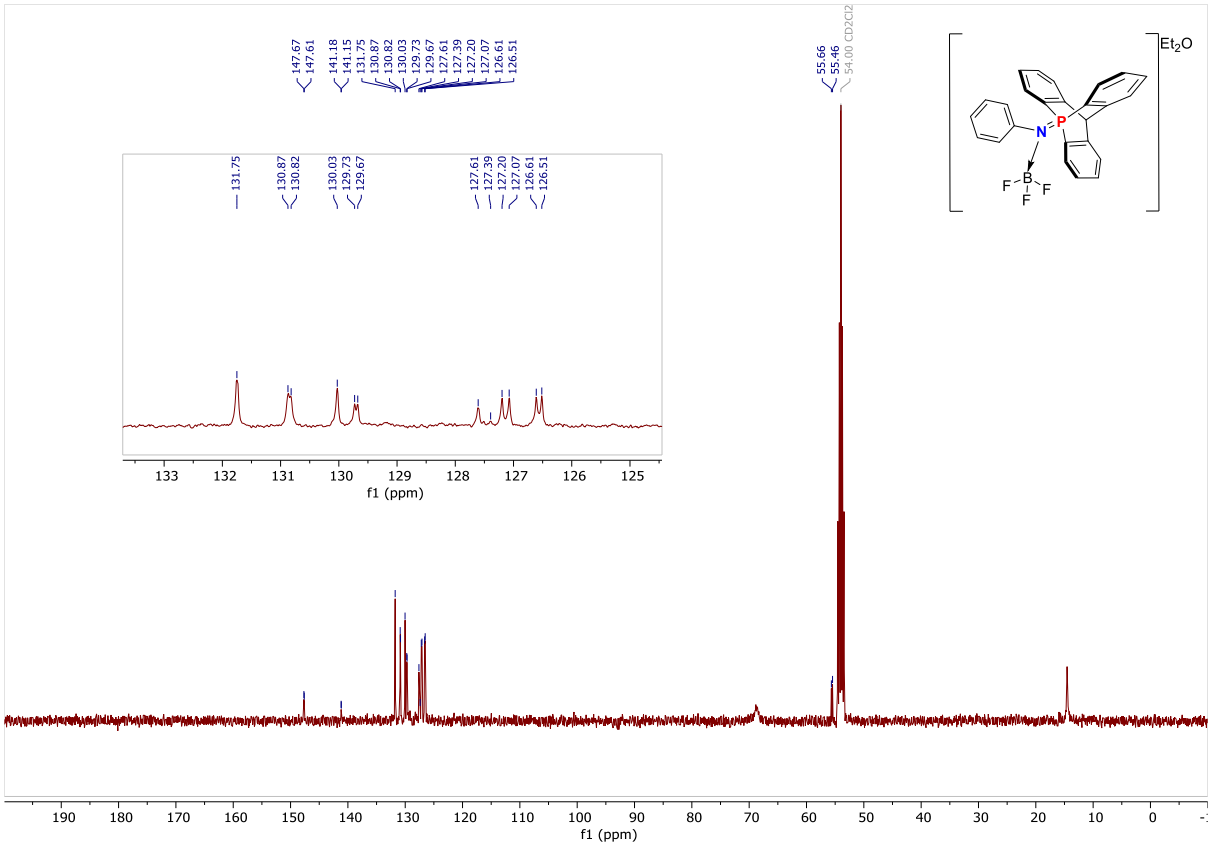
^{31}P NMR (202 MHz, 25 °C, $CDCl_3$) of **15**



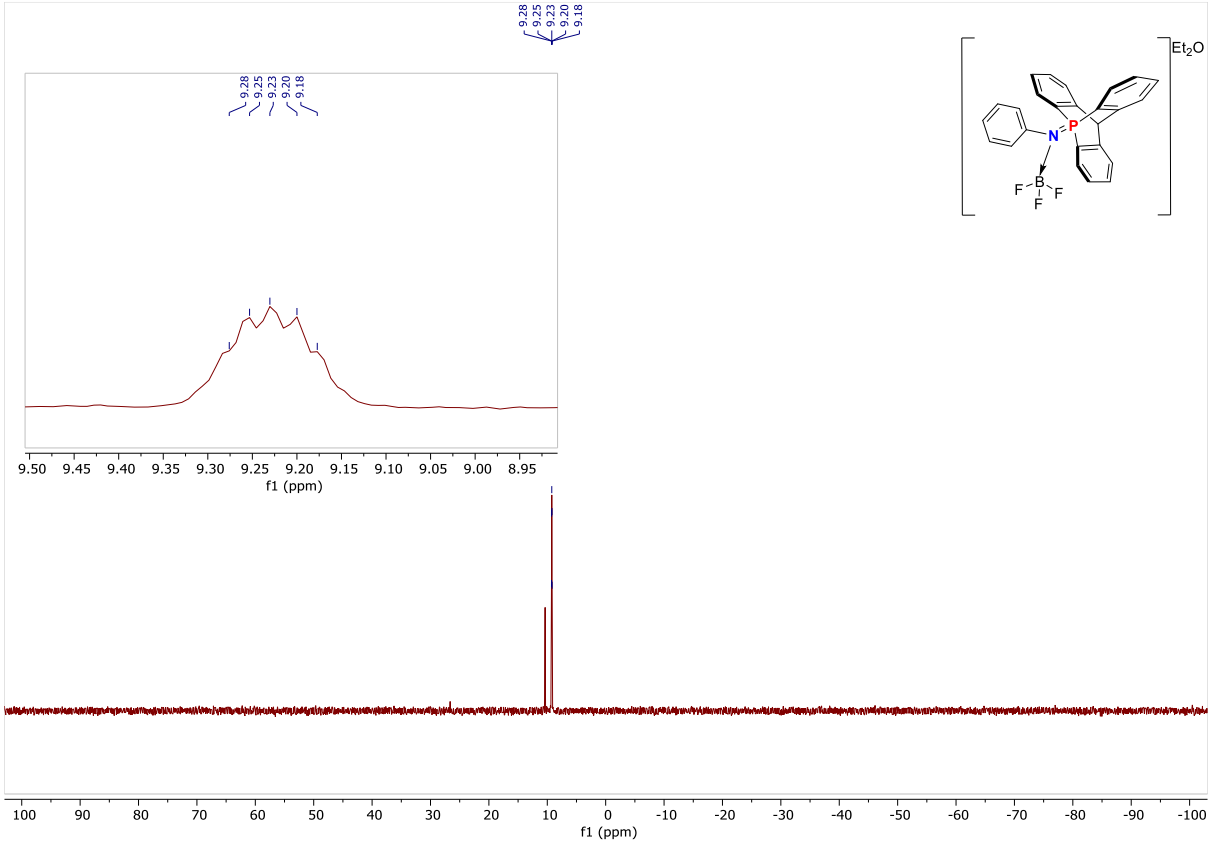
^{19}F NMR (471 MHz, 25 °C, $CDCl_3$) of **15**



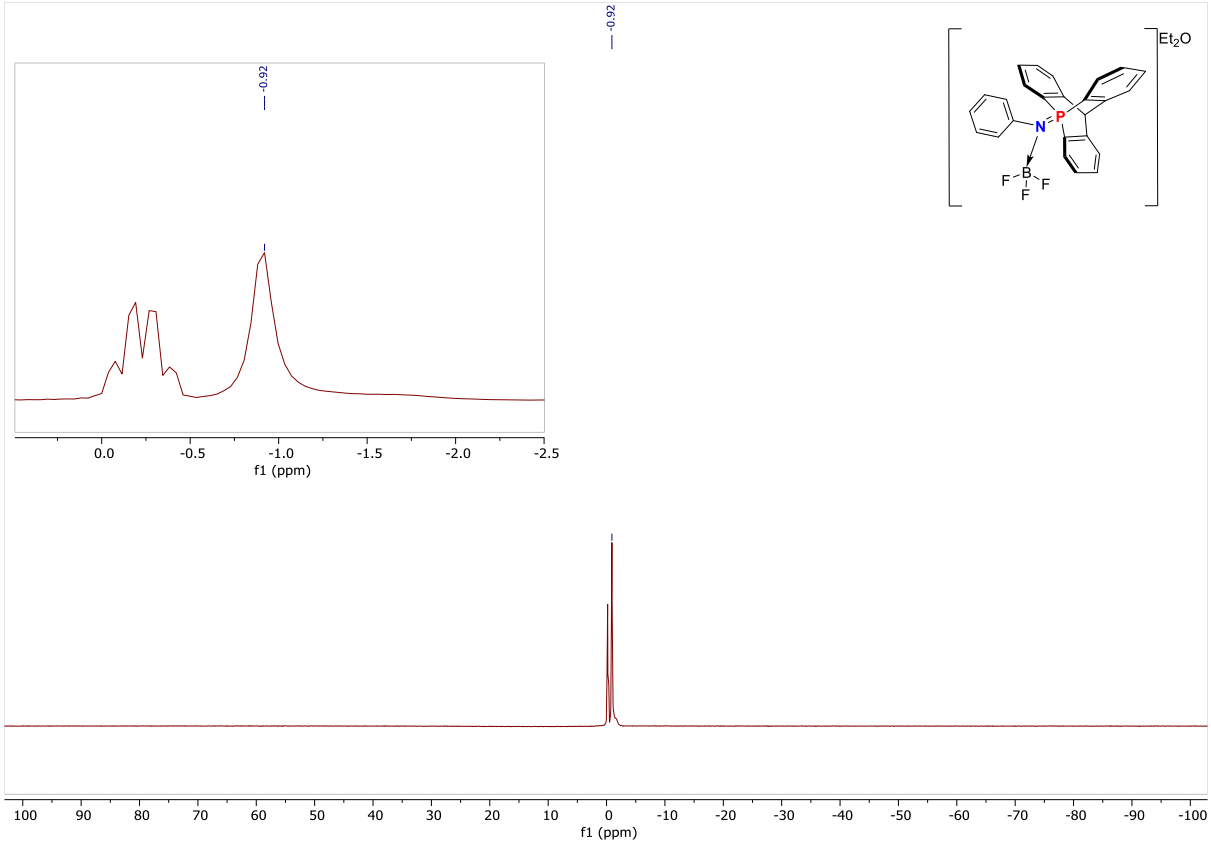
^{1}H NMR (400 MHz, 25 °C, CD_2Cl_2) of **16**



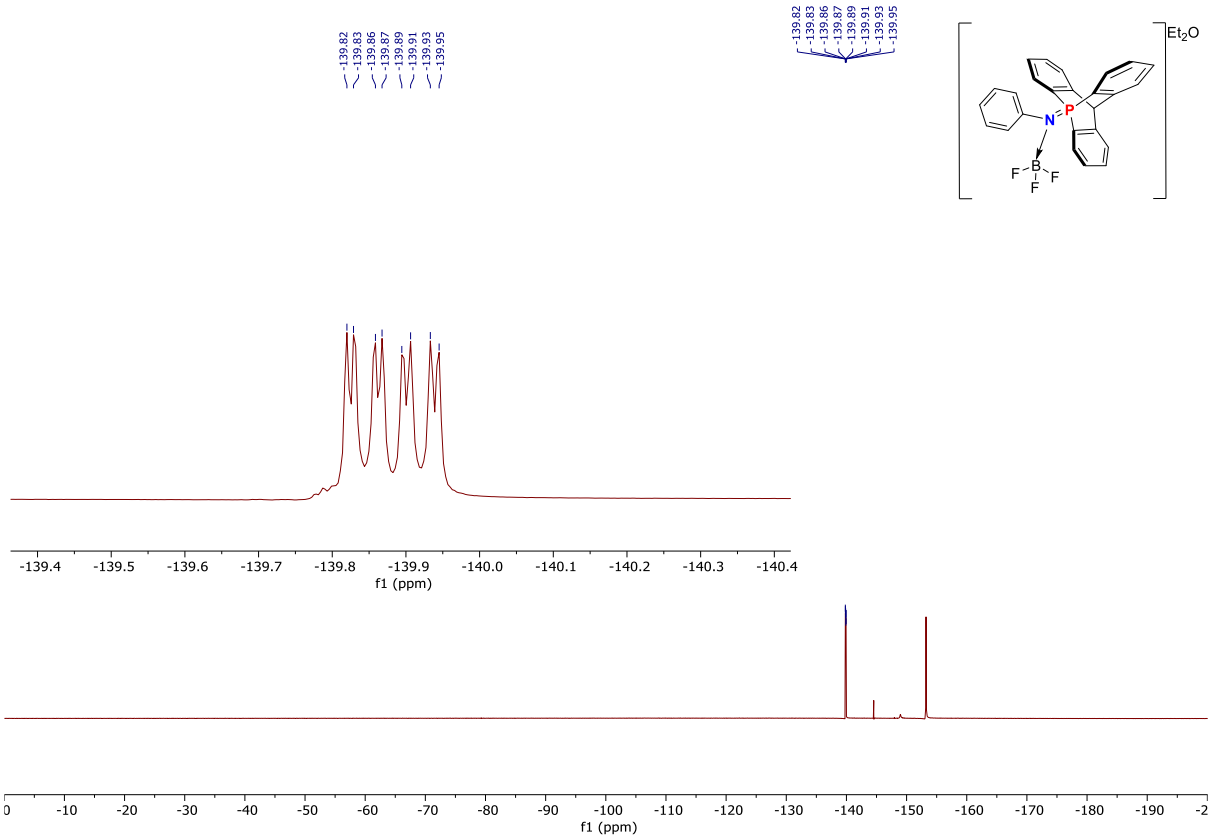
^{13}C NMR (101 MHz, 25 °C, CD_2Cl_2) of **16**



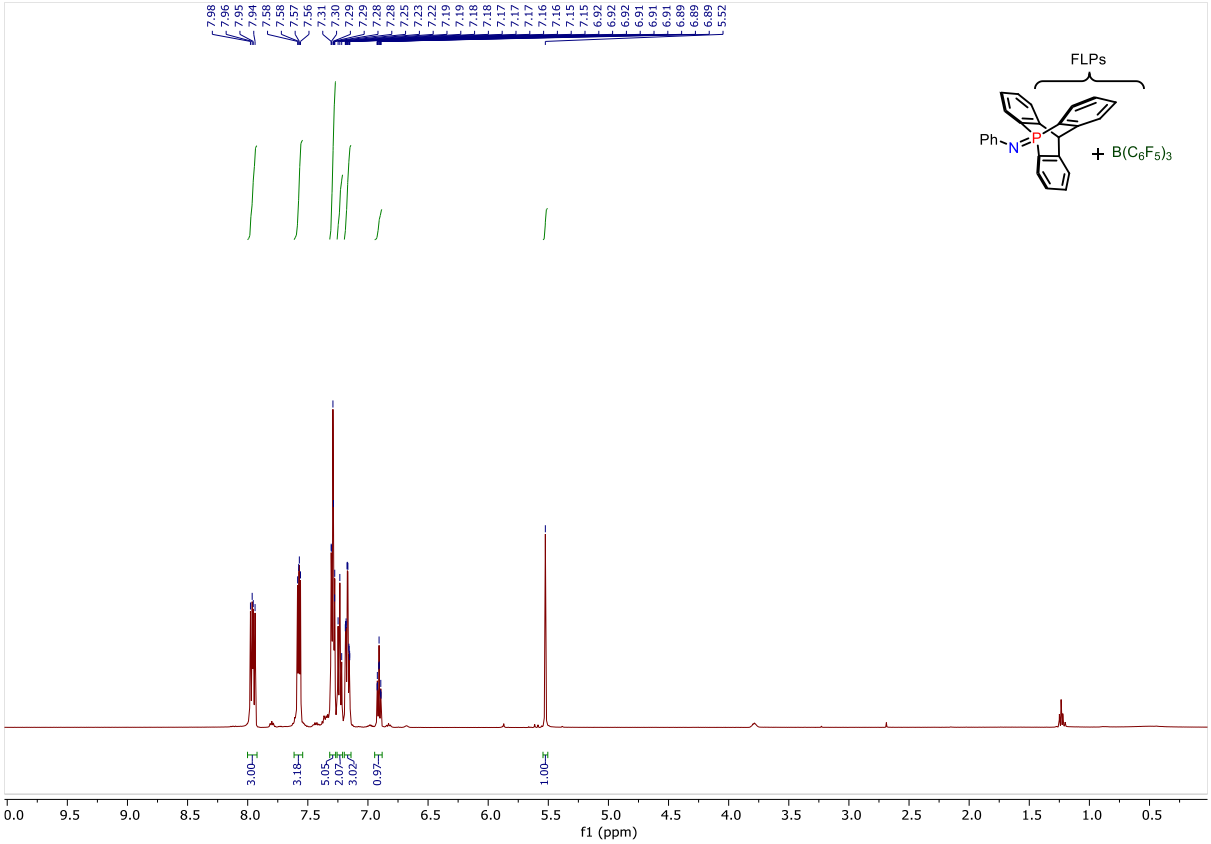
^{31}P NMR (202 MHz, 25 °C, CD_2Cl_2) of **16**



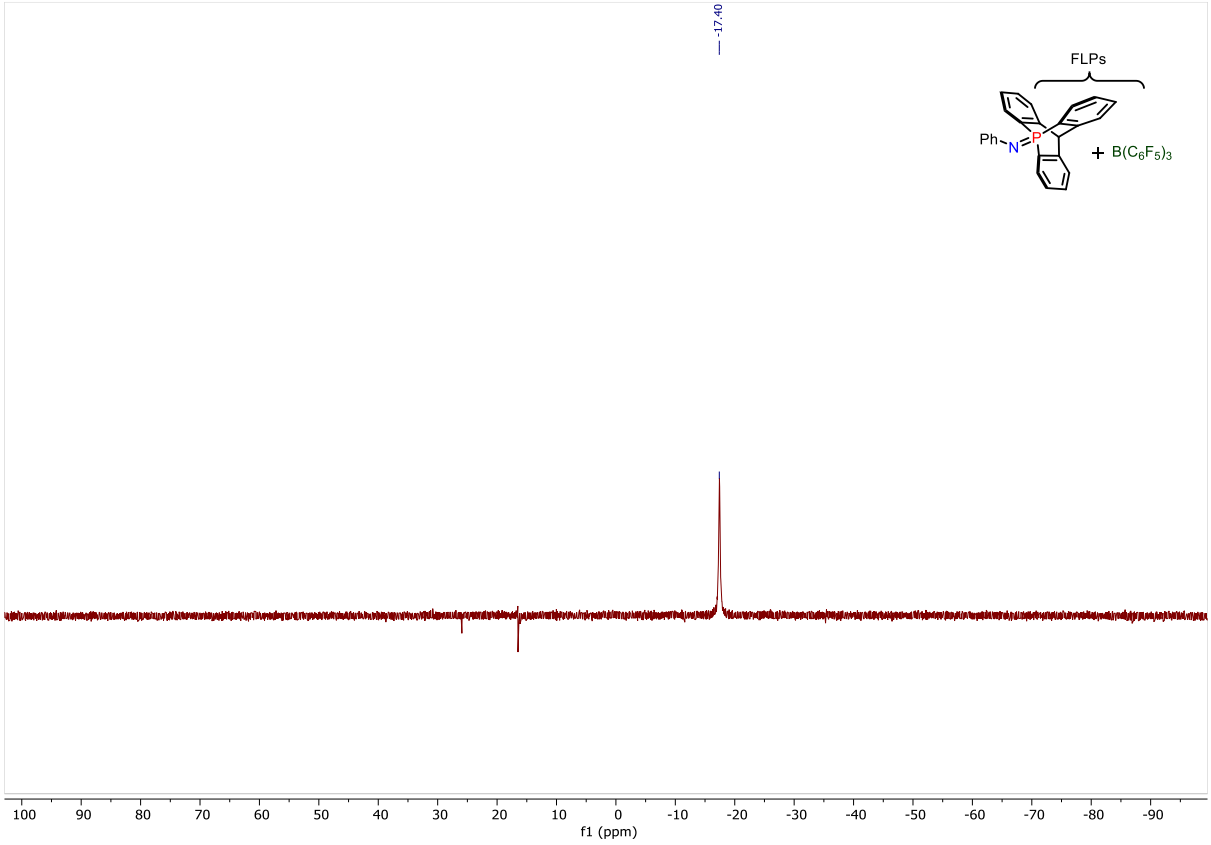
^{11}B NMR (160 MHz, 25 °C, CD_2Cl_2) of **16**



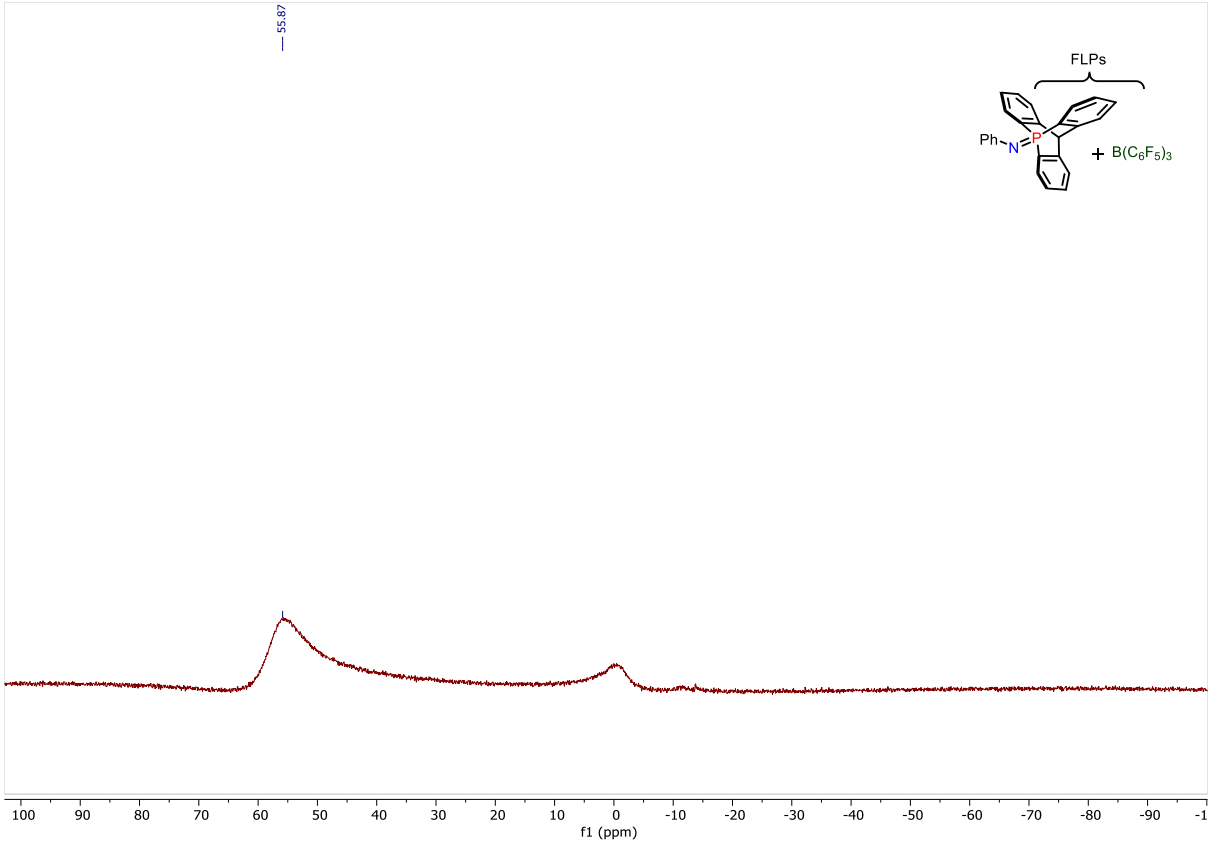
^{19}F NMR (471 MHz, 25 °C, CD_2Cl_2) of **16**



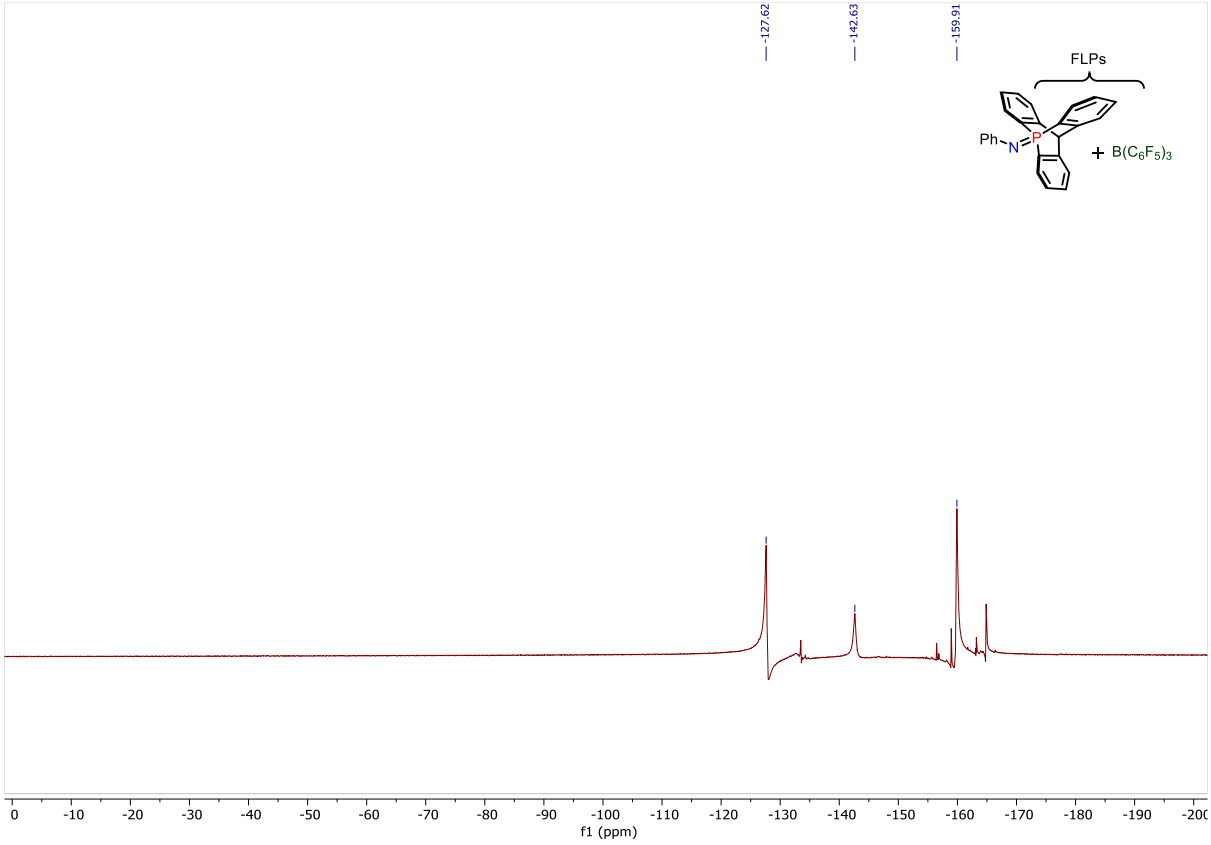
^{1}H NMR (500 MHz, 25 °C, $CDCl_3$) of the FLP between **13** and **17**.



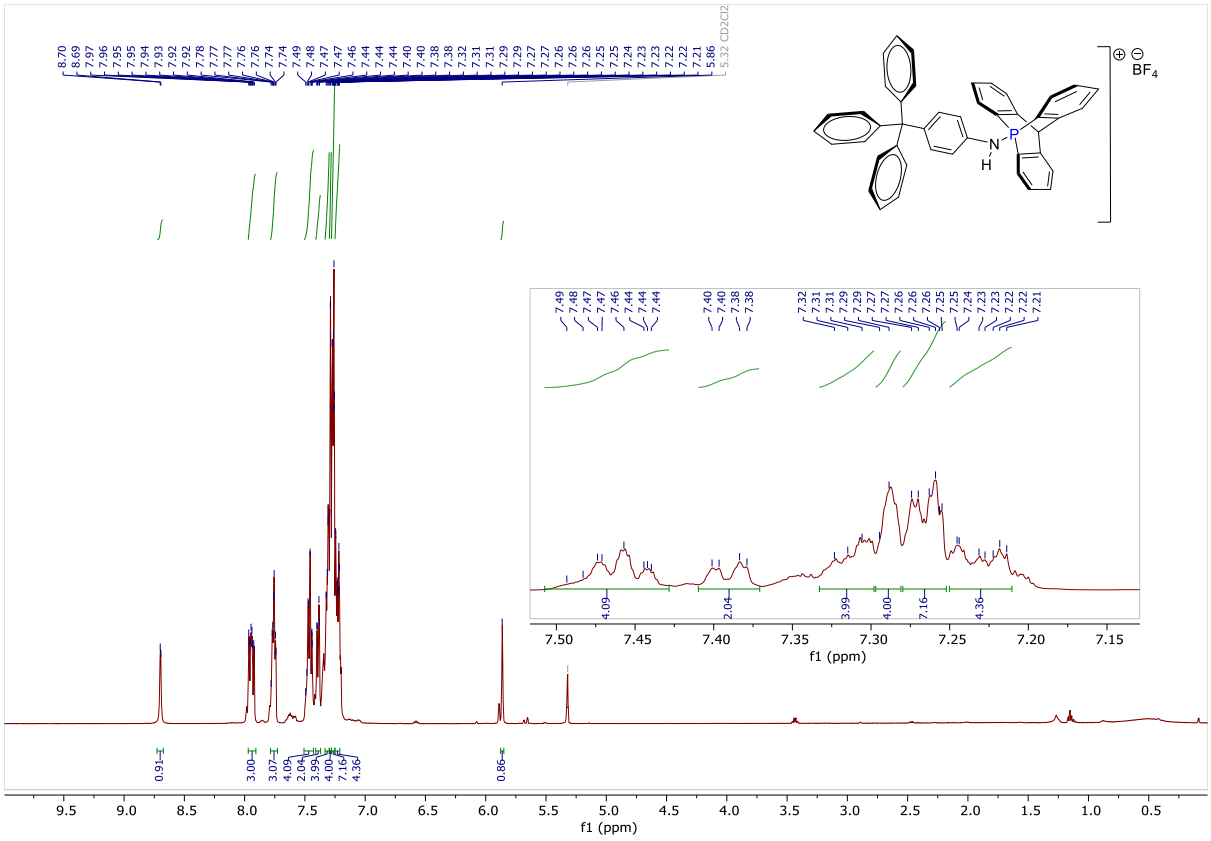
^{31}P NMR (202 MHz, 25 °C, $CDCl_3$) of the FLP between **13** and **17**.



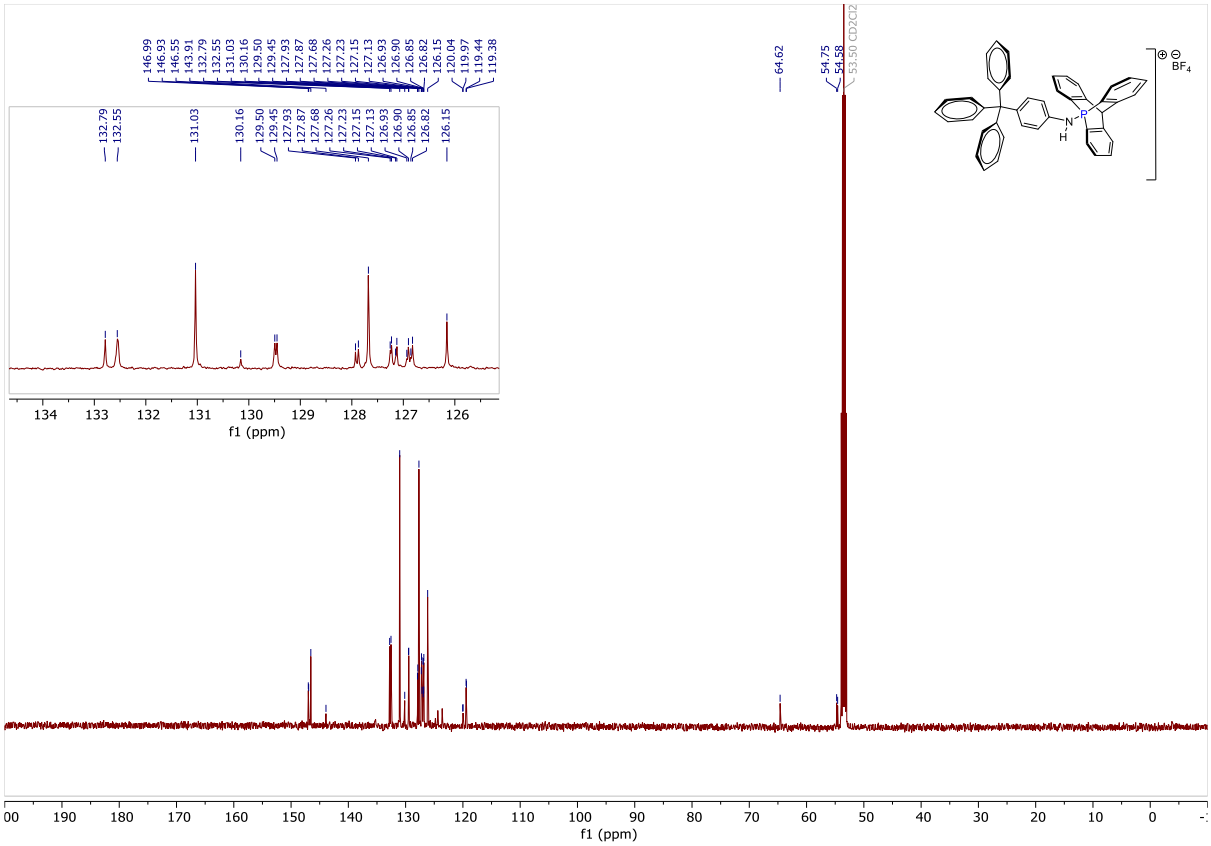
^{11}B NMR (160 MHz, 25 °C, $CDCl_3$) of the FLP between **13** and **17**.



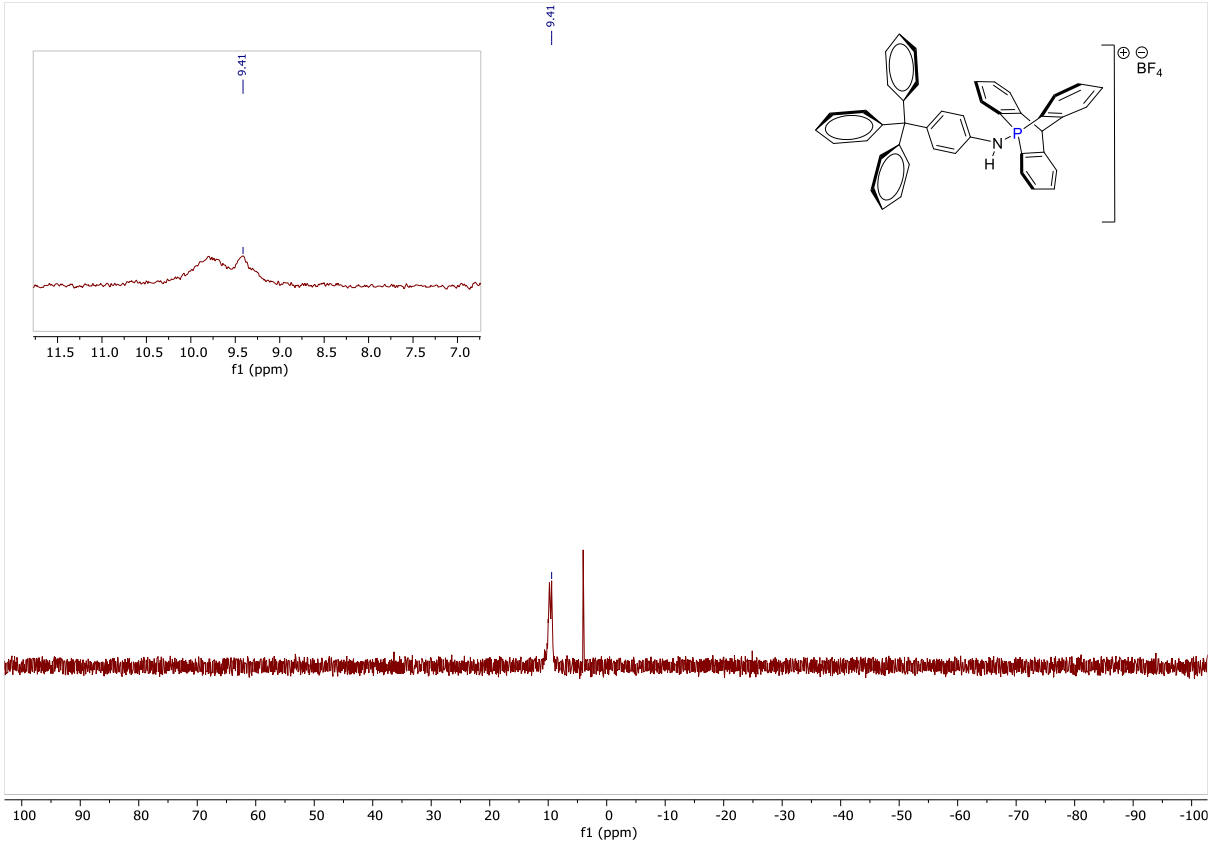
^{19}F NMR (471 MHz, 25 °C, $CDCl_3$) of the FLP between **13** and **17**.



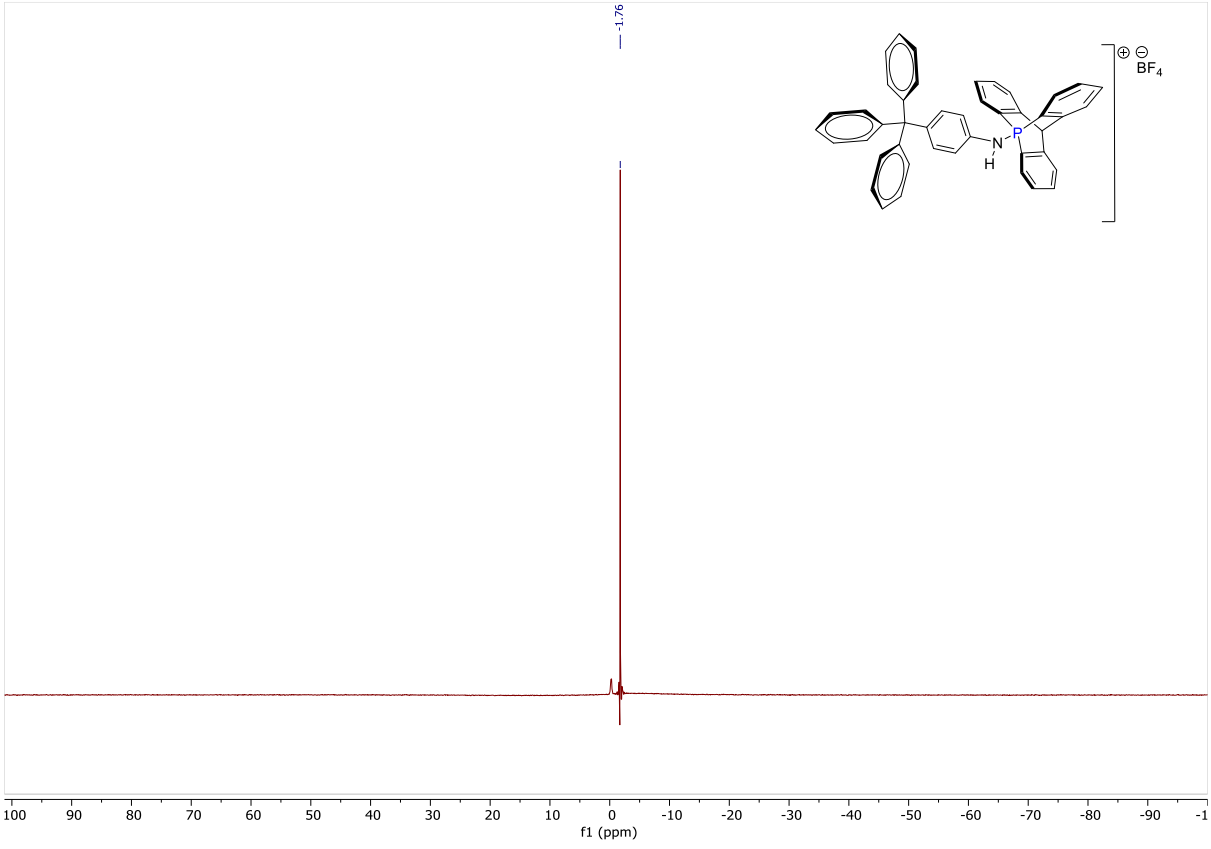
^{1}H NMR (500 MHz, 25 °C, CD_2Cl_2) of **20**.



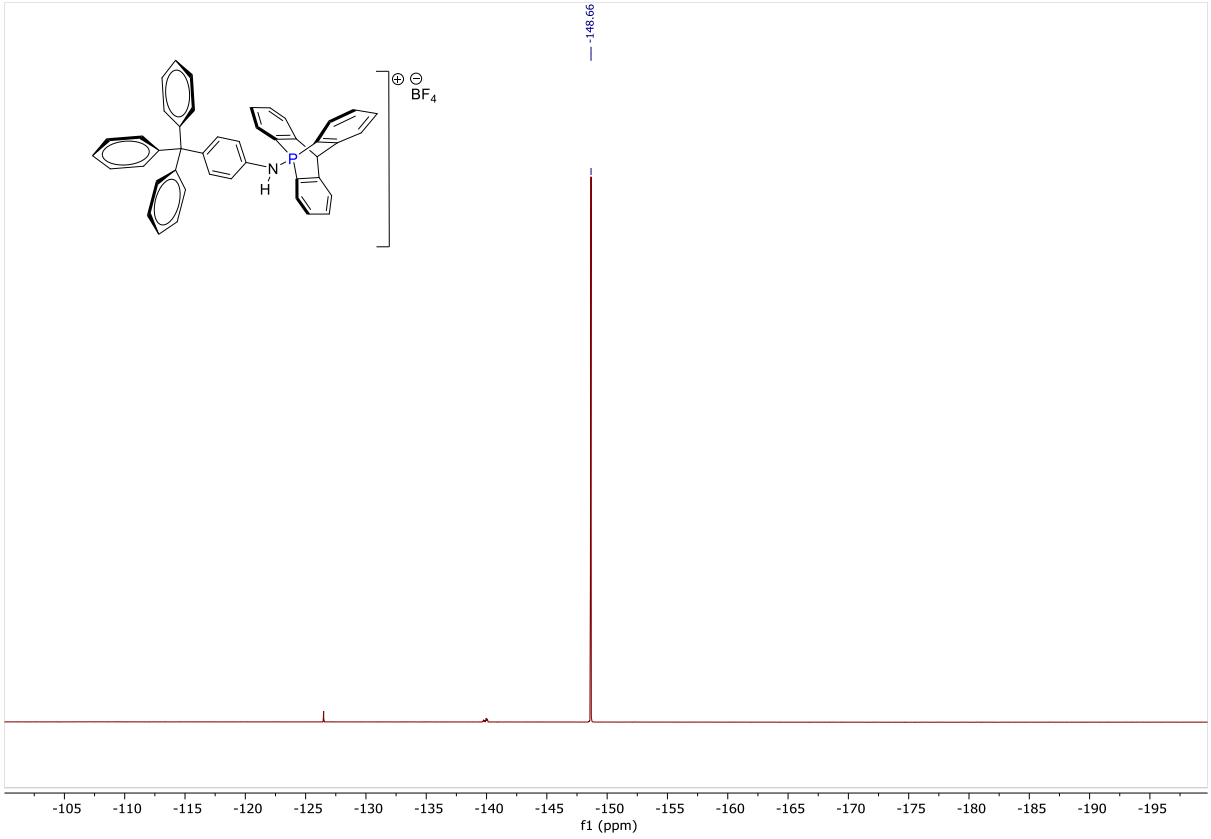
^{13}C NMR (126 MHz, 25 °C, CD_2Cl_2) of **20**



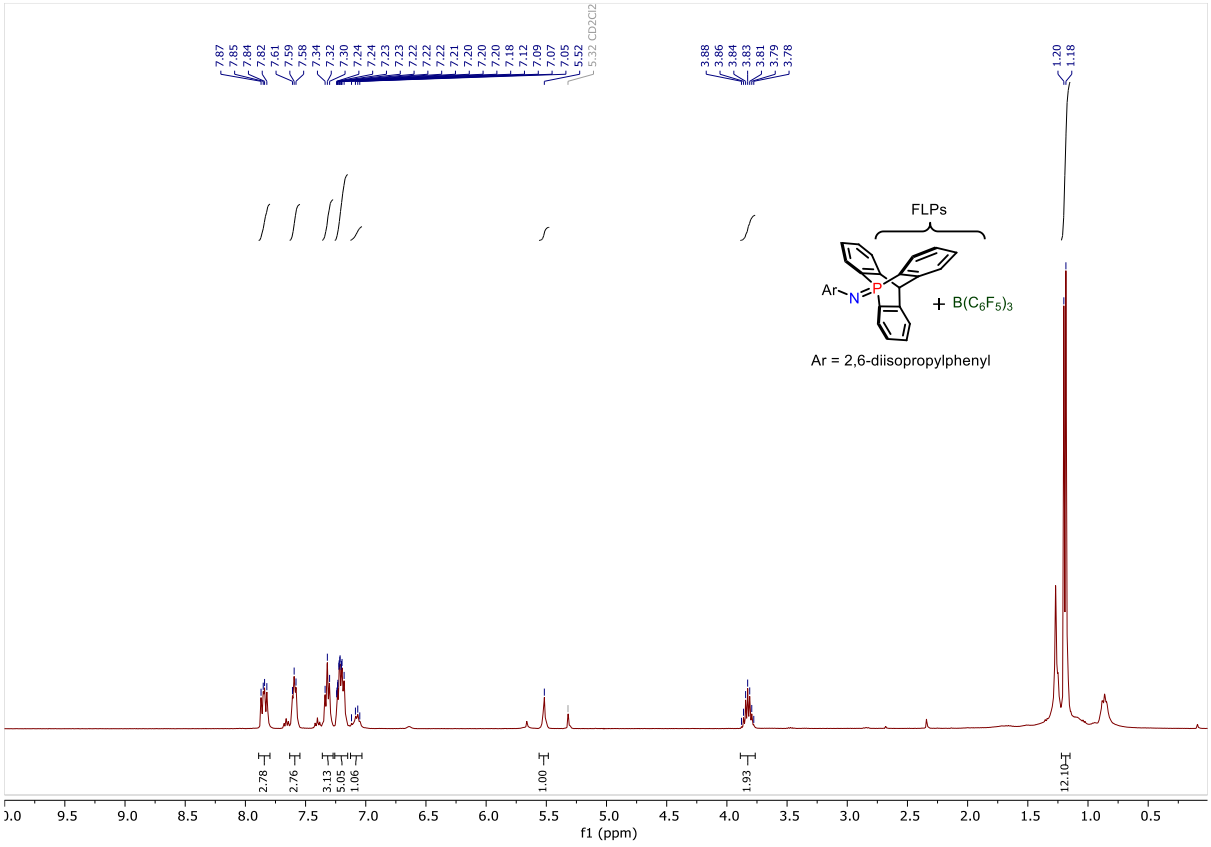
^{31}P NMR (202 MHz, 25 °C, CD_2Cl_2) of **20**



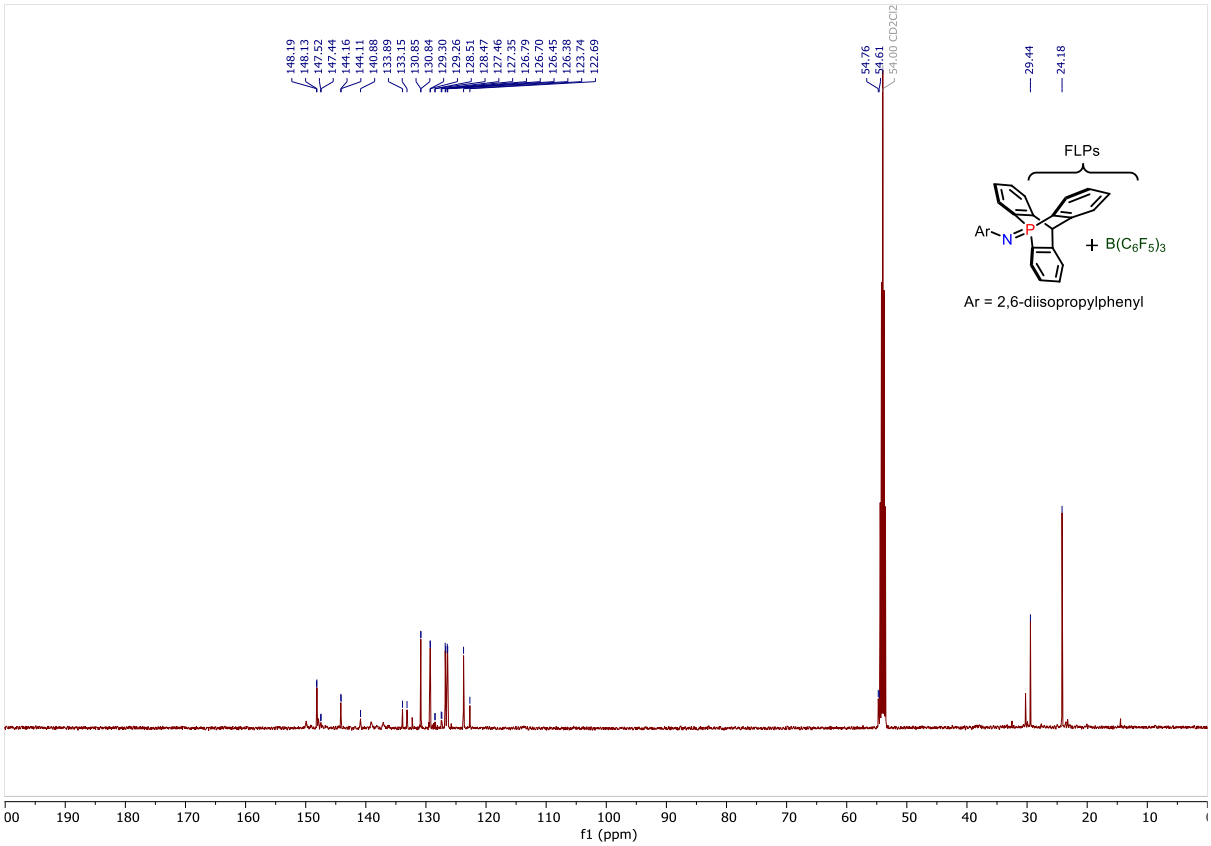
^{11}B NMR (160 MHz, 25 °C, CD_2Cl_2) of **20**



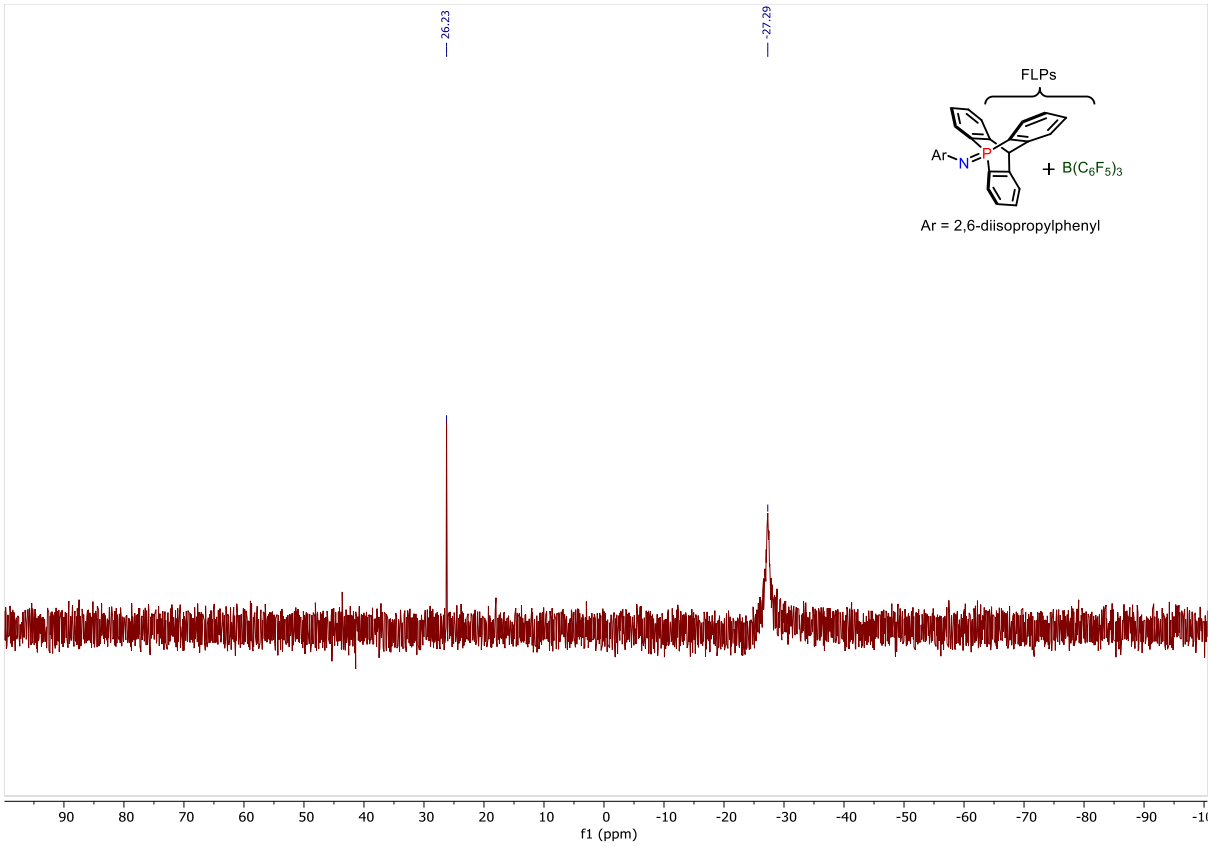
^{19}F NMR (471 MHz, 25 °C, CD_2Cl_2) of **20**



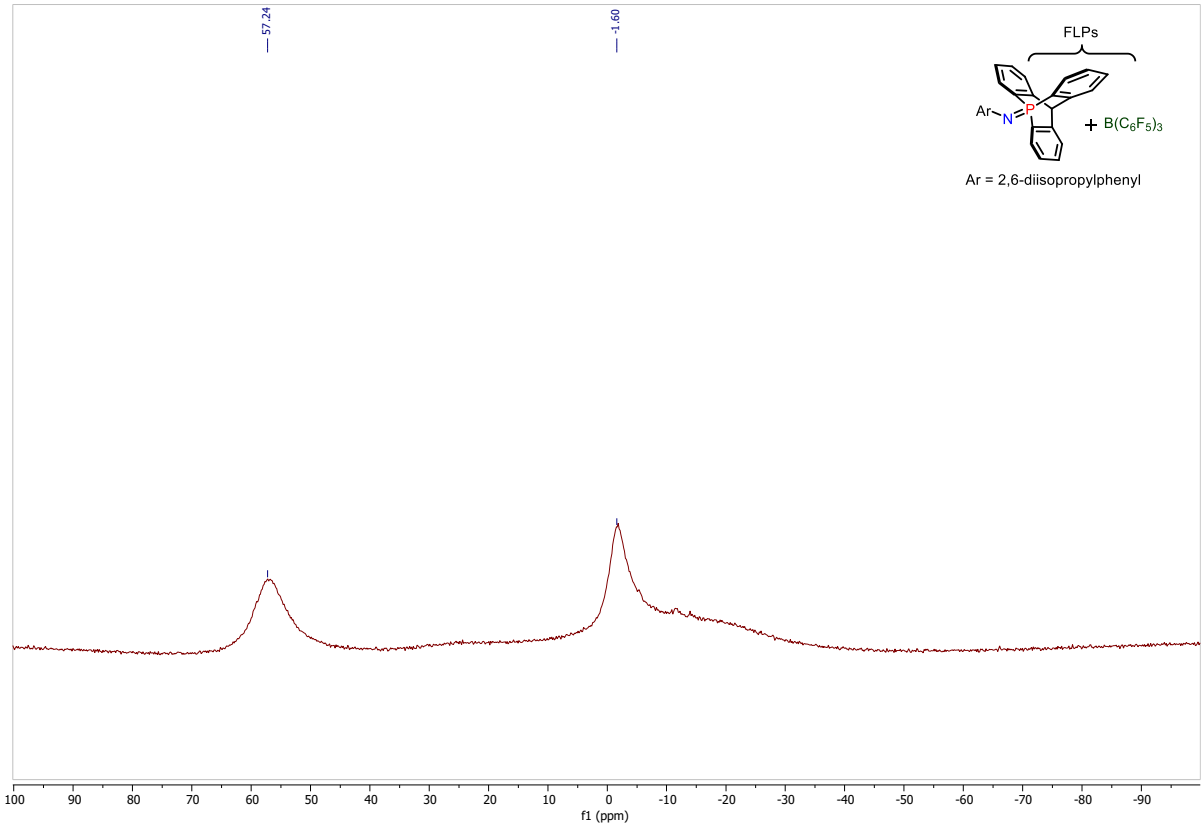
^{1}H NMR (400 MHz, 25 °C, CD_2Cl_2) of **21**



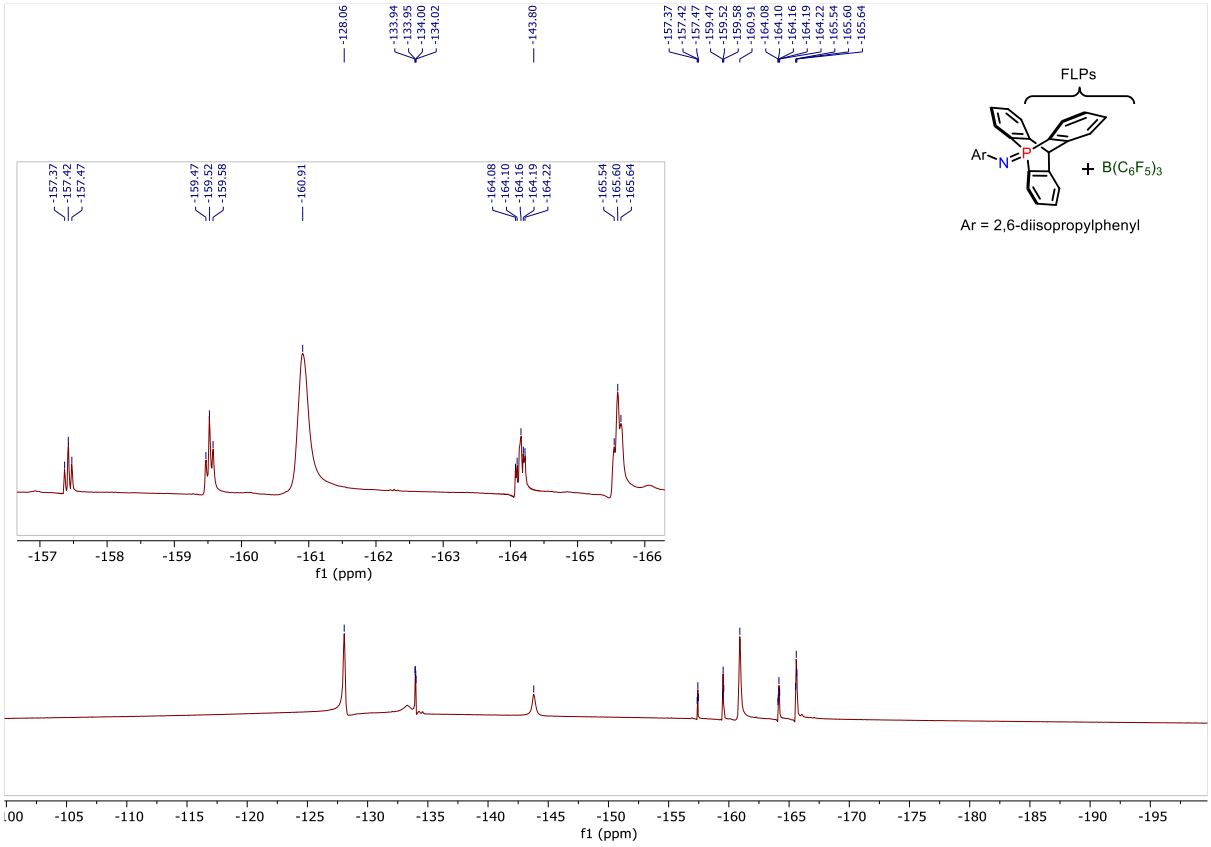
^{13}C NMR (126 MHz, 25 °C, CD_2Cl_2) of **21**



^{31}P NMR (162 MHz, 25 °C, CD_2Cl_2) of **21.**



^{11}B NMR (128 MHz, 25 °C, CD_2Cl_2) of **21**



^{19}F NMR (376 MHz, 25 °C, CD_2Cl_2) of **21**

5. Crystallographic data

Diffraction data were collected using the Oxford Diffraction Gemini R Ultra (Cu Kα with multilayer mirrors or Mo Kα with graphite monochromator, Ruby CCD area detector) and Bruker D8 Venture (Cu Kα or Ag Kα microsource, multilayer mirror, Photon III C14 detector) diffractometers. Data collection, unit cells determination and data reduction were carried out using CrysAlis PRO software package[3] and APEX4 software package[x] using Olex2[4] and shelXle[5a], the structure was solved with the SHELXT 2015[3b] structure solution program by Intrinsic Phasing methods and refined by full-matrix least squares on $|F|^2$ using SHELXL-2018/3[3b]. Non-hydrogen atoms were refined anisotropically. Most of hydrogen atoms were located from electron density map. In most cases, hydrogen atoms, not involved in hydrogen bonding, were placed on calculated positions in riding mode with temperature factors fixed at 1.2 times U_{eq} of the parent carbon atoms (1.5 times for methyl groups). Details of the data collection and refinement are given in the table below.

The compound **6** reported in Table 1 was found to stabilize a molecule of H_2O_2 in the solid-state by interacting through two hydrogen bonds as shown below. It also crystalized with or without molecules of water as shown in Table S1.

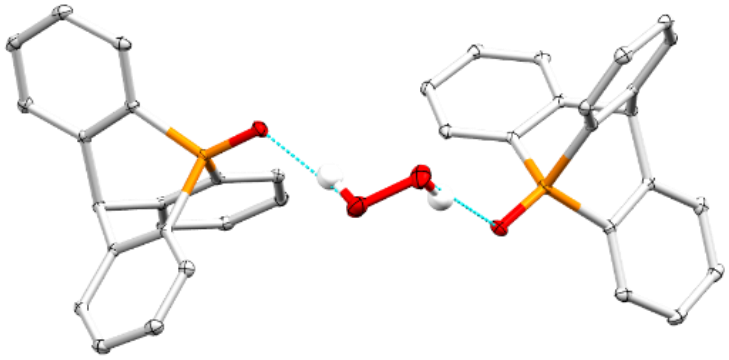


Figure S1. Ellipsoid representation of single crystal X-ray structure of **6** in the presence of H_2O_2 molecule showing the two hydrogen bonds between the OH groups of H_2O_2 and two P=O oxides functionalities of molecule **6.** Ellipsoid values are at 50% probability level, H-atoms in the molecule are omitted for clarity.

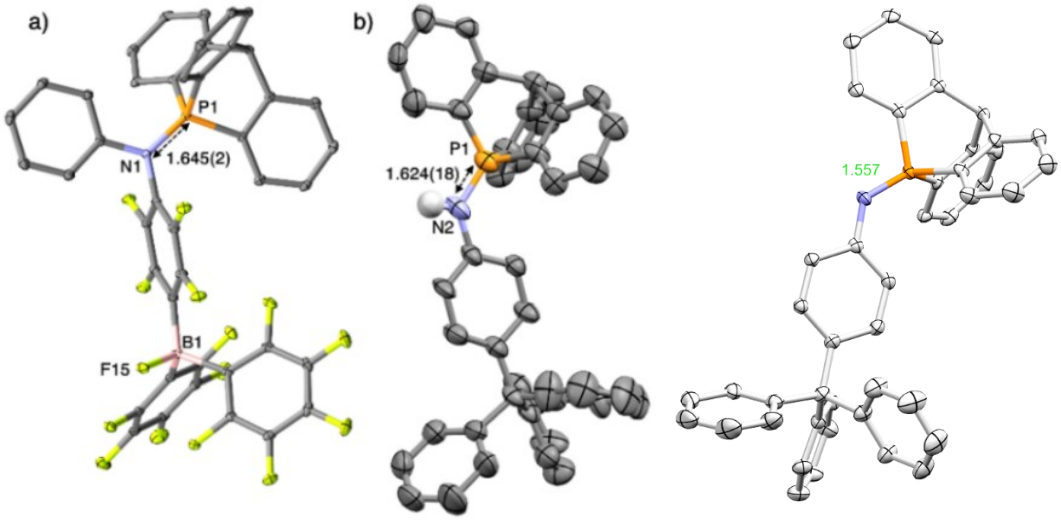


Figure S2: Ellipsoid representation (50% probability level) of single-crystal X-ray structures of **18** (a), and **21** (b). H atoms, anion and solvent omitted for clarity. For the structure of the neutral form of compound **21** (right) see structure CCDC 2353832.

Table S1. Experimental crystallographic details

	6	**6·½H₂O**	**6·½H₂O LT**	**6·½H₂O₂**
Chemical formula	$C_{19}H_{13}OP$	$2(C_{19}H_{13}OP)\cdot H_2O$	$2(C_{19}H_{13}OP)\cdot H_2O$	$C_{19}H_{13}OP\cdot 0.5(H_2O_2)$
M_r	288.26	594.54	594.54	305.27
Crystal system, space group	Triclinic, $P\bar{1}$	Orthorhombic, *Pbca*	Orthorhombic, *Pbca*	Monoclinic, *C*2/*c*
Temperature (K)	100	295	100	100
a, *b*, *c* (Å)	7.2774 (2), 8.0944 (3), 13.1388 (4)	16.51047 (10), 16.41081 (10), 23.08005 (14)	16.3712 (2), 16.2810 (2), 22.9501 (3)	20.3958 (6), 13.4454 (6), 12.1945 (4)
α, β, γ (°)	81.7506 (9), 79.8049 (10), 70.6319 (9)	90, 90, 90	90, 90, 90	90, 117.604 (1), 90
V (Å^3)	715.63 (4)	6253.54 (7)	6117.11 (13)	2963.44 (19)
Z	2	8	8	8
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	1.65	1.55	1.58	1.68
Crystal size (mm)	0.36 × 0.26 × 0.07	0.44 × 0.31 × 0.14	0.24 × 0.22 × 0.11	0.29 × 0.18 × 0.13
Diffractometer	Bruker D8 Venture	Oxford Diffraction Gemini Ultra R	Bruker D8 Venture	
Absorption correction	Numerical	Analytical	Numerical	
T_{min}, T_{max}	0.637, 1.000	0.641, 0.864	0.58, 0.84	0.59, 0.81
No. of measured, independent and observed reflections	27465, 2579, 2578 [$I > 2\sigma(I)$]	28008, 5550, 5212 [$I > 2\sigma(I)$]	47278, 5577, 4794 [$I > 2\sigma(I)$]	24650, 2676, 2671 [$I > 2\sigma(I)$]
R_{int}	0.036	0.019	0.050	0.047
θ_{max} (°)	68.2	67.1	68.2	68.1
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.602	0.598	0.602	0.602
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.086, 1.12	0.034, 0.097, 1.07	0.052, 0.146, 1.11	0.035, 0.089, 1.08
No. of reflections	2579	5550	5577	2676
No. of parameters	380	980	980	204
No. of restraints	391	1047	1099	0
H-atom treatment	constrained			mixed
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e·Å^{-3})	0.27, -0.45	0.18, -0.23	0.31, -0.30	0.41, -0.32
CCDC deposition number	2347266	2313762	2347267	2347268

	7	**7 (LT)**	**8**	**8 (LT)**
Chemical formula	$C_{19}H_{13}PS$	$C_{19}H_{13}PS$	$C_{19}H_{13}PSe$	$C_{19}H_{13}PSe$
M_r	304.32	304.36	351.22	351.22
Crystal system, space group	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*
Temperature (K)	297	100	297	100
a, *b*, *c* (Å)	14.2480 (3), 13.5359 (3), 15.8127 (3)	14.0811 (3), 13.4388 (3), 15.6879 (4)	14.1963 (6), 13.7375 (6), 15.8281 (7)	14.0369 (5), 13.6803 (5), 15.7202 (5)
α, β, γ (°)	90, 90.772 (1), 90	90, 90.464 (1), 90	90, 90.897 (1), 90	90, 90.789 (1), 90
V (Å^3)	3049.35 (11)	2968.57 (12)	3086.4 (2)	3018.45 (18)
Z	8	8	8	8
Radiation type	Cu *K*α	Cu *K*α	Ag *K*α, λ = 0.56086 Å	Ag *K*α, λ = 0.56086 Å
μ (mm^{-1})	2.77	2.85	1.34	1.37
Crystal size (mm)	0.13 × 0.11 × 0.05	0.22 × 0.19 × 0.18	0.47 × 0.29 × 0.18	0.29 × 0.27 × 0.12
Diffractometer	Bruker D8 Venture			
Absorption correction	Numerical			
T_{min}, T_{max}	0.772, 1.000	0.772, 1.000	0.265, 0.465	0.61, 0.85
No. of measured, independent and observed reflections	22816, 2701, 2431 [$I > 2\sigma(I)$]	42618, 2716, 2685 [$I \geq 2u(I)$]	40566, 3150, 2866 [$I > 2\sigma(I)$]	17865, 2661, 2503 [$I > 2\sigma(I)$]
R_{int}	0.041	0.040	0.053	0.056
θ_{max} (°)	66.7	68.2	20.5	19.5
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.596	0.602	0.625	0.595
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.034, 0.093, 1.08	0.015, 0.036, 1.10	0.039, 0.104, 1.09	0.029, 0.078, 1.08
No. of reflections	2701	2716	3150	2661
No. of parameters	190	307	190	190
No. of restraints	0	0	0	0
H-atom treatment	constrained			
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e·Å^{-3})	0.28, -0.26	0.19, -0.18	0.67, -0.33	0.60, -0.34
CCDC deposition number	2313763	2313764	2313765	2347269

	9	**10**	**11**	**12**
Chemical formula	$C_{26}H_{20}NO_2PS$	$C_{24}H_{22}NOP$	$C_{31}H_{23}NO_3P_2$	$C_{34}H_{36}NO_2PS$
M_r	441.46	371.39	519.44	553.67
Crystal system, space group	Monoclinic, $P2_1/c$	Orthorhombic, $Pna2_1$	Monoclinic, $P2_1/c$	Orthorhombic, $P2_12_12_1$
Temperature (K)	295	295	100	100
a, b, c (Å)	8.19512 (14), 13.9420 (2), 19.4641 (3)	17.31590 (19), 9.40206 (10), 12.48870 (13)	11.81181 (13), 19.91502 (17), 11.98573 (13)	9.31097 (12), 12.97197 (17), 24.0692 (5)
α, β, γ (°)	90, 99.7093 (16), 90	90, 90, 90	90, 118.9392 (15), 90	90, 90, 90
V (Å^3)	2192.04 (7)	2033.23 (4)	2467.38 (5)	2907.12 (8)
Z	4	4	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	2.19	1.28	1.89	0.20
Crystal size (mm)	0.46 × 0.22 × 0.15	0.50 × 0.24 × 0.04	0.49 × 0.30 × 0.04	0.59 × 0.24 × 0.11
Diffractometer	Oxford Diffraction Gemini Ultra R			
Absorption correction	Analytical			
T_{min}, T_{max}	0.508, 0.740	0.610, 0.955	0.557, 0.923	0.915, 0.984
No. of measured, independent and observed reflections	11121, 3893, 3579 [$I > 2\sigma(I)$]	9451, 3147, 3017 [$I > 2\sigma(I)$]	17799, 4379, 4054 [$I > 2\sigma(I)$]	40245, 10003, 8710 [$I > 2\sigma(I)$]
R_{int}	0.028	0.022	0.025	0.039
θ_{max} (°)	67.1	67.1	67.0	32.9
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.597	0.597	0.597	0.763
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.183, 1.09	0.035, 0.098, 1.06	0.032, 0.083, 1.01	0.041, 0.096, 1.02
No. of reflections	3893	3147	4379	10003
No. of parameters	281	248	434	494
No. of restraints	0	1	121	216
H-atom treatment	constrained			
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e·Å^{-3})	0.91, -0.62	0.26, -0.18	0.30, -0.34	0.30, -0.33
Absolute structure	–	Refined as an inversion twin.	–	Flack x determined using 3322 quotients.
Absolute structure parameter	–	0.32 (3)	–	-0.02 (2)
CCDC deposition number	2313766	2313767	2313768	2313769

	13	**14**	**15**	**16**
Chemical formula	$C_{25}H_{18}NP$	$C_{31}H_{30}NP$	$C_{25}H_{19}NP{\cdot}C_2F_6NO_4S_2$	$C_{25}H_{18}BF_3NP{\cdot}0.5(CH_2Cl_2)$
M_r	363.37	447.53	644.53	473.65
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$
Temperature (K)	100	100	100	100
a, b, c (Å)	8.9413 (2), 13.6176 (3), 15.5673 (4)	9.0484 (3), 18.3060 (6), 14.4219 (4)	8.3718 (3), 17.3368 (6), 20.1621 (8)	9.5904 (2), 16.0488 (3), 14.2154 (3)
α, β, γ (°)	90, 90, 90	90, 90.4144 (18), 90	113.9252 (10), 91.4063 (12), 93.9353 (11)	90, 101.406 (1), 90
V (Å^3)	1895.46 (8)	2388.78 (13)	2664.18 (17)	2144.74 (8)
Z	4	4	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Ag $K\alpha$, λ = 0.56086 Å	Cu $K\alpha$
μ (mm^{-1})	1.33	1.15	0.18	2.64
Crystal size (mm)	0.37 × 0.16 × 0.02	0.20 × 0.12 × 0.02	0.46 × 0.34 × 0.24	0.37 × 0.12 × 0.02
Diffractometer	Bruker D8 Venture			
Absorption correction	Numerical			
T_{min}, T_{max}	0.705, 1.000	0.76, 0.98	0.923, 1.000	0.581, 1.000
No. of measured, independent and observed reflections	46523, 3881, 3865 [$I > 2\sigma(I)$]	23060, 4145, 3529 [$I > 2\sigma(I)$]	151281, 16187, 14930 [$I > 2\sigma(I)$]	21498, 3919, 3813 [$I > 2\sigma(I)$]
R_{int}	0.065	0.053	0.061	0.037
θ_{max} (°)	74.5	66.8	23.6	68.3
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.596	0.715	0.603
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.101, 1.19	0.078, 0.177, 1.15	0.045, 0.125, 1.05	0.045, 0.115, 1.13
No. of reflections	3881	4145	16187	3919
No. of parameters	245	386	1029	317
No. of restraints	0	201	404	26
H-atom treatment	constrained			
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e·Å^{-3})	0.46, -0.26	0.52, -0.38	0.60, -0.38	0.41, -0.39
Absolute structure	Refined as an inversion twin.	–	–	–
Absolute structure parameter	0.14 (3)	–	–	–
CCDC deposition number	2313770	2347270	2313771	2313772

	18	**20**
Chemical formula	$C_{43}H_{18}BF_{15}NP\cdot CH_2Cl_2$	$C_{44}H_{33}NP^{+}\cdot BF_4^{-}$
M_r	960.29	693.49
Crystal system, space group	Triclinic, $P\bar{1}$	Orthorhombic, $Pca2_1$
Temperature (K)	100	296
a, b, c (Å)	11.2365 (2), 12.2624 (2), 14.8185 (3)	12.867 (4), 13.069 (4), 21.505 (6)
α, β, γ (°)	83.390 (1), 78.060 (1), 74.601 (1)	90, 90, 90
V (Å^3)	1921.98 (6)	3616.2 (18)
Z	2	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	2.92	1.11
Crystal size (mm)	0.28 × 0.11 × 0.07	0.04 × 0.03 × 0.02
Diffractometer	Bruker D8 Venture	
Absorption correction	Numerical	Multi-scan .
T_{min}, T_{max}	0.616, 1.000	0.568, 1.000
No. of measured, independent and observed reflections	71257, 7031, 6547 [$I > 2\sigma(I)$]	3086, 2459, 1312 [$I > 2\sigma(I)$]
R_{int}	0.054	0.034
θ_{max} (°)	68.3	48.2
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.602	0.484
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.090, 1.03	0.079, 0.230, 1.04
No. of reflections	7031	2459
No. of parameters	605	461
No. of restraints	25	379
H-atom treatment	constrained	
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e·Å^{-3})	0.65, -0.33	0.22, -0.30
Absolute structure	–	Flack x determined using 330 quotients.
Absolute structure parameter	–	0.03 (7)
CCDC deposition number	2313773	2313774

6. Computational methods

Computations have been carried out using the Jaguar 8.5 pseudospectral program package.[6] All species have been fully geometry optimized, and the Cartesian coordinates are supplied in the next section. PA and MCA values are calculated at the M06-2X/6-311+G(d,p)/ /M06-2X/6-31+G(d) level as the difference in enthalpy at 298 K between the neutral and the protonated and methylated imine, respectively.

Fluoride ion affinities (FIAs) are estimated at the M06-2X/6-311+G(d,p)//M06-2X/6-31+G(d) level using isodesmic approach with COF_2 anchor point as described by Christe;[7] subtraction of the enthalpies of eq. 2 from eq. 1 providing the absolute FIA (Table S2).

$$\begin{array}{rl} CF_3O^- + LA \rightarrow COF_2 + LAF^- & \text{eq. 1} \\ \underline{CF_3O^- \rightarrow COF_2 + F^-} & \text{eq. 2 } (\Delta H_{exp} = 49.9 \text{ kcal mol}^{-1})^{8} \\ LA + F^- \rightarrow LAF^- & \end{array}$$

For comparison, FIAs were also computed according to the method described by Greb[9] using the following isodesmic reactions: $Me_3SiF + LA \rightarrow Me_3Si^+ + LAF^-$ and $Me_3SiF \rightarrow Me_3Si^+ + F^-$ with the enthalpy value of 227.9 kcal mol^{-1} for the second reaction (Table S2, bottom line).

Table S2. Computed FIA values (in kcal mol^{-1}).

	Cmpd B	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**Ph_3P=NPh**
FIA (COF_2 system)	60	30	27	30	47	37	45	51	36	38	32
FIA (TMS-system)	73	43	40	44	60	50	58	64	49	51	45

NBO analysis was performed using the NBO 6.0 program[10] as implemented in Jaguar.

As described by N. Fey,[11] the He_8_steric parameters were computed by optimizing the phosphoratriptycene imine geometries at the BP86/6-31+G(d) level, its nitrogen atom constrained to lie at 1.7 or 2.2 Å above the centroid, and perpendicular to the plane, of a helium ring which is constituted by eight helium atoms with a 2.5 Å radius (see Figure S3 for 5). Reported relative energies values correspond to electronic energies obtained at the BP86/6-31G(d) level.

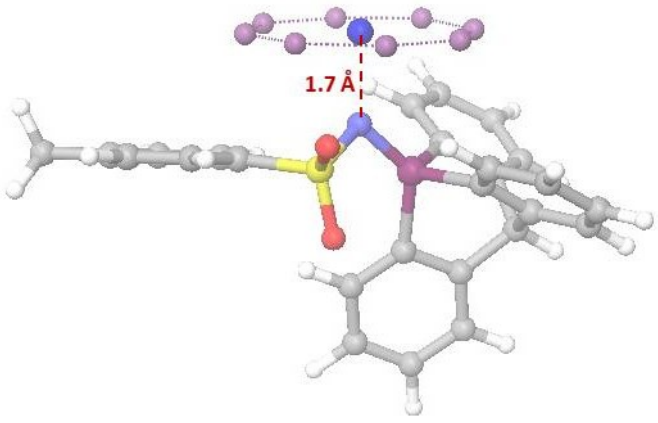


Figure S3. Geometric model used for computation of the He_8_steric parameter illustrated for **13**.

Percent buried volume[12] and steric contour maps were determined using the SambVca 2.1 application.[12] The metal was defined as the center of the sphere and the N atom of the nitrogen ylide derivatives being analyzed was used to define the -*z*-axis (Figures S4 and S5). The following default parameters were used for all calculations: atomic radii were the bond radii scaled by 1.17; sphere radius = 3.5 Å, mesh spacing = 0.1 Å, and H atoms were excluded from the calculations.

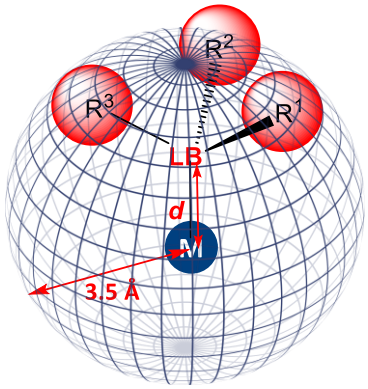


Figure S4. Description of the method applied to calculate the $\%V_{bur}$ parameter.

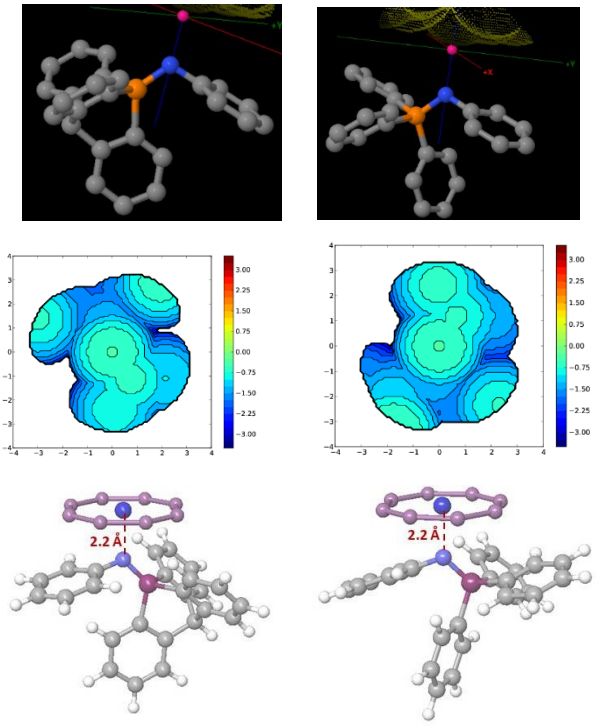


Figure S5. Steric parameters calculations for TripP=NPh **13** (left) and for its analogue Ph_3P=NPh (right). Top: Geometric models used for computation of their buried volumes; Middle: topographic steric maps with a M-N distance of 1.7 Å. Bottom: geometric models used for computation of their He_8_steric parameters.

Table S3. Computed steric He_8_steric parameters (kcal mol^{-1}) and buried volume ($\%V_{bur}$) at two different N-centroid distances for phosphatriptycene imines **9-14** and for the reference triphenylphosphine-iminophosphorane Ph_3P=NPh.

Steric parameters	**9**	**10**	**11**	**12**	**13**	**14**	**Ph_3P=NPh**
He_8_steric 1.70 Å	42	50	43	51	25	35	24
He_8_steric 2.20 Å	22	29	23	28	13	16	15
$\%V_{bur}$[a] 1.70 Å	32.8	34.6	31.3	35.7	32.1	35.2	32.3
$\%V_{bur}$[a] 2.20 Å	28.5	28.4	28.4	30.4	26.2	28.1	26.0

[a] $\%V_{bur}$ computed using the SambVca with the solid-state input geometries. Hydrogen atoms are excluded, and sphere radius set at 3.5 Å. N-centroid distances of 1.7 and 2.2 Å. Atomic radii default, scaled bond radii of 1.17 Å, see the ESI for detailed calculations.

The difference in FIA between **13** and Ph_3P=NPh was analyzed through the distortion/Interaction-activation strain model of Houk and Bickelhaupt (Table S4).[13]

Table S4. Fluoride anion affinities (FIA), distortion (ΔE_{strain}) and interaction (ΔE_{int}) energies (in kcal.mol^{-1}) calculated at the M06-2X/6-311+G(d,p) level.

	13	**Ph_3P=NPh**
FIA	36	32
ΔE_{strain}	27.9	32.5
ΔE_{int}	-73.2	-71.9

These results indicate that the slight enhancement of Lewis acidity at the phosphorus atom (as evidenced by FIA) with geometric constraints is mainly due to a lower distortion energy. The energy necessary for the triptycene structure in **13** to adopt the trigonal bipyramidal geometry is indeed lower (by 4.6 kcal mol^{-1}) than the one required for Ph_3P=NPh.

7. Structures and energies

He8_ring

E(BP86/6-31G*) = -23.15522221938

He1 2.4999755124 0.0000000000 0.0000000000
He2 -2.4999755124 0.0000000000 0.0000000000
He3 0.0000000000 2.4999755124 0.0000000000
He4 0.0000000000 -2.4999755124 0.0000000000
He5 1.7677496376 1.7677496376 0.0000000000
He6 -1.7677496376 -1.7677496376 0.0000000000
He7 -1.7677496376 1.7677496376 0.0000000000
He8 1.7677496376 -1.7677496376 0.0000000000
X9 -0.0000500000 0.0000125000 0.0000000000

6

E(M06-2X/6-311+G**) = -1148.32482818063
H(M06-2X/6-31+G*) = -1148.11876483316

C1	-2.4910593056	1.2650121164	6.9598985999
C2	-2.7924019883	2.5580860312	6.5210027336
C3	-1.7840331328	3.5020298788	6.3434013783
C4	-0.4540847071	3.1622031287	6.6035955862
C5	-0.1612843976	1.8764989488	7.0384642670
C6	1.4257102944	-0.2795257210	6.4551070269
C7	2.3941735235	-0.7078581038	5.5570560396
C8	2.2024718735	-1.9147811979	4.8798211126
C9	1.0541882907	-2.6684775717	5.1096188573

C10	0.0826654072	-2.2317651383	6.0156454394
C11	0.2655204934	-1.0330085665	6.6933994436
C12	-1.1712260650	0.9187618527	7.2210091304
H13	-3.2847665606	0.5345512816	7.0963234967
H14	-3.8247991899	2.8269244639	6.3174828816
H15	-2.0312683525	4.5028020263	6.0026910951
H16	0.3482675915	3.8831188747	6.4709581965
H17	3.2826453972	-0.1040496451	5.3926204974
H18	2.9496306430	-2.2652082893	4.1743390664
H19	0.9094628420	-3.6061771635	4.5811210343
H20	-0.8106693183	-2.8267119279	6.1893910964
C21	0.3185669095	-0.6882934901	11.3992333896
C22	1.4401160394	0.1371787753	11.3977224485
C23	1.8501904823	0.7577460743	10.2149619309
C24	1.1239421931	0.5370740664	9.0524580298
C25	-0.0077911651	-0.2935851059	9.0445868744
C26	-0.4084603349	-0.9066353110	10.2249240083
H27	0.0030487608	-1.1687297117	12.3207190360
H28	1.9964771096	0.2989416865	12.3158622725
H29	2.7224609913	1.4055466911	10.1920519758
H30	-1.2828343986	-1.5525203388	10.2348003014
C31	-0.7280326847	-0.4621602838	7.7060282031
H32	-1.5904066693	-1.1260813400	7.8147197961
P33	1.5023566499	1.2552431333	7.4259004056
O34	2.6771552843	2.1609547009	7.2777374186

6-H$^+$

E(M06-2X/6-311+G**) = -1148.68633374365

H(M06-2X/6-31+G*) = -1148.47394069304

C1	-2.4674799915	1.2863452009	6.9514493984
C2	-2.7607602135	2.5812272148	6.5123991166
C3	-1.7537575633	3.5276457661	6.3358983945
C4	-0.4240896539	3.1948036760	6.5970479214
C5	-0.1489133516	1.9044074553	7.0327412465
C6	1.4538679132	-0.2983378941	6.4401322997
C7	2.4180467219	-0.7194696241	5.5317320807
C8	2.2110358781	-1.9239076667	4.8585388518
C9	1.0596444434	-2.6700704908	5.0992587171
C10	0.0929208594	-2.2316951010	6.0092479371
C11	0.2822615247	-1.0372040284	6.6904114689
C12	-1.1515639222	0.9340169605	7.2170832182
H13	-3.2644784111	0.5602764435	7.0840666451
H14	-3.7914574082	2.8514912517	6.3061303848
H15	-2.0009614315	4.5271324464	5.9945713865
H16	0.3717219116	3.9213559494	6.4643826025
H17	3.3075913401	-0.1271632883	5.3362158350
H18	2.9480464651	-2.2754394601	4.1444825992
H19	0.9069145883	-3.6052387200	4.5701334627
H20	-0.8028729512	-2.8215821335	6.1814444534
C21	0.3100721784	-0.6917988444	11.4082531343
C22	1.4311682861	0.1347606285	11.4254071054
C23	1.8580068899	0.7596641132	10.2531794662
C24	1.1415906574	0.5280271074	9.0848814470
C25	0.0029665759	-0.2985649692	9.0516121476
C26	-0.4079834237	-0.9089425607	10.2284433149
H27	-0.0154242758	-1.1724409749	12.3252765283
H28	1.9728215356	0.2980084600	12.3509365040
H29	2.7231627615	1.4166581878	10.2639942796

H30	-1.2844067786	-1.5503952568	10.2325827617
C31	-0.7110463910	-0.4545535968	7.7029938901
H32	-1.5767236474	-1.1121165179	7.8056815369
P33	1.4230848542	1.1793968455	7.4448889568
O34	2.6129934738	2.2161490001	7.2642799392
H35	3.5201943309	1.9114410867	7.4390885132

6-Me$^+$

E(M06-2X/6-311+G**) = -1187.97702531867

H(M06-2X/6-31+G*) = -1187.75977845225

C1	-2.4630657348	1.2963705743	6.9518059990
C2	-2.7509696306	2.5868733630	6.4964620240
C3	-1.7394126340	3.5255887020	6.3058217360
C4	-0.4111652052	3.1880499360	6.5690269412
C5	-0.1406312209	1.9022464663	7.0206356628
C6	1.4431972806	-0.3183152342	6.4522293791
C7	2.3954903809	-0.7507220585	5.5360063099
C8	2.1738672148	-1.9554160816	4.8679294445
C9	1.0186851665	-2.6917884353	5.1201853222
C10	0.0625033636	-2.2419189962	6.0356569357
C11	0.2676808770	-1.0468829561	6.7116072593
C12	-1.1485316639	0.9397975680	7.2195279144
H13	-3.2636103642	0.5761747121	7.0955024845
H14	-3.7808319754	2.8593977604	6.2887701807
H15	-1.9818806322	4.5218944039	5.9519781688
H16	0.3886589282	3.9080250319	6.4255134322
H17	3.2878590624	-0.1655889110	5.3325835175
H18	2.9018719742	-2.3148676865	4.1485085451
H19	0.8539476946	-3.6270879209	4.5948044981

H20	-0.8379049751	-2.8226164219	6.2152257186
C21	0.3069571725	-0.6444782567	11.4270792822
C22	1.4324665651	0.1764481377	11.4324116455
C23	1.8612739840	0.7825784022	10.2510575906
C24	1.1436582080	0.5395972381	9.0850891860
C25	0.0003165258	-0.2803183459	9.0655879782
C26	-0.4132725793	-0.8731995314	10.2507975974
H27	-0.0200265899	-1.1115735736	12.3505786647
H28	1.9752855291	0.3496043815	12.3554976211
H29	2.7308488916	1.4337545268	10.2514973039
H30	-1.2940313547	-1.5090737326	10.2642410132
C31	-0.7176340809	-0.4464608253	7.7210812691
H32	-1.5889400330	-1.0951385603	7.8330779257
P33	1.4324259555	1.1767070429	7.4371195732
O34	2.6401726658	2.1722152257	7.2504118005
C35	4.0147366810	1.7907015106	7.5290728416
H36	4.3874000241	2.4731485044	8.2918041590
H37	4.0746162006	0.7561123564	7.8786539639
H38	4.5751684572	1.9136176133	6.6032713248

6-F^-

E(M06-2X/6-311+G**) = -1248.2272147024

H(M06-2X/6-31+G*) = -1247.99033663496

C1	0.0345627362	-1.5787176455	6.3886142816
C2	0.0286920239	-1.5593569704	4.9931073006
C3	0.2787209381	-0.3671678544	4.3142297644
C4	0.5471580853	0.8005565466	5.0294563258
C5	0.5358362181	0.7892786858	6.4216639746

C6	1.8957471258	1.4885730961	8.8001132616
C7	3.0266020088	2.0736445869	9.3634204023
C8	3.7405192004	1.4083270042	10.3608469937
C9	3.3408537238	0.1380289697	10.7748288031
C10	2.2184273100	-0.4596868658	10.1997036839
C11	1.4874835040	0.2143415861	9.2228070599
C12	0.2757150470	-0.4079966328	7.1057564846
H13	-0.1615804877	-2.5065705173	6.9235410413
H14	-0.1700900311	-2.4734197381	4.4387044870
H15	0.2795340392	-0.3506997931	3.2268700339
H16	0.7846503752	1.7275260710	4.5141395646
H17	3.3507222927	3.0453759441	9.0003876961
H18	4.6178729816	1.8734203035	10.8041486312
H19	3.9016158533	-0.3886701820	11.5433545963
H20	1.9019966045	-1.4509903918	10.5203151032
C21	-2.9959769072	1.2666536054	9.9821846801
C22	-2.8149553209	2.5616422549	9.4994858173
C23	-1.6753328463	2.8844101823	8.7526817196
C24	-0.7083890574	1.9195361401	8.4822080250
C25	-0.9071721006	0.6242625742	8.9757321890
C26	-2.0334325485	0.2868757231	9.7184427385
H27	-3.8817503964	1.0162528388	10.5618730788
H28	-3.5650184758	3.3230590702	9.7054362496
H29	-1.5140974544	3.8876868079	8.3657621369
H30	-2.1644642928	-0.7288467565	10.0904879878
C31	0.2068131753	-0.3532696155	8.6257786278
H32	0.0063327975	-1.3507256997	9.0337312754
O33	0.6026005581	3.7462174033	7.1932080957
P34	0.9082747924	2.2850302464	7.4497981951
F35	2.4348828513	2.3505889951	6.5584132145

7^{-}

E(M06-2X/6-311+G**) = -1471.29670755109

H(M06-2X/6-31+G*) = -1471.08176633123

C1	-2.4762705389	1.2703344722	6.9729009249
C2	-2.7797373722	2.5629366532	6.5353392672
C3	-1.7722371485	3.5077982842	6.3585965914
C4	-0.4418834386	3.1694093858	6.6183205920
C5	-0.1486202822	1.8846021074	7.0518044569
C6	1.4401371574	-0.2743557221	6.4691097031
C7	2.4082817642	-0.7034507380	5.5729133543
C8	2.2154808544	-1.9105425961	4.8964522802
C9	1.0664750978	-2.6630114132	5.1259382968
C10	0.0956147568	-2.2241218025	6.0310049965
C11	0.2789526544	-1.0249008783	6.7081649031
C12	-1.1560158054	0.9249794382	7.2339093336
H13	-3.2682883777	0.5379954842	7.1092774787
H14	-3.8125940355	2.8303605352	6.3325082790
H15	-2.0198173856	4.5087903483	6.0190813808
H16	0.3614584844	3.8903750324	6.4874791760
H17	3.2974158844	-0.0991750205	5.4099600360
H18	2.9630884394	-2.2614438132	4.1918190278
H19	0.9206741462	-3.6009768128	4.5983039500
H20	-0.7988440887	-2.8172065433	6.2054133678
C21	0.3255895057	-0.6883977682	11.4103213623
C22	1.4474191076	0.1364858860	11.4120880866
C23	1.8595243023	0.7598652395	10.2316318907
C24	1.1348022604	0.5415981048	9.0689145457
C25	0.0028593775	-0.2876742253	9.0557946809

C26	-0.3996113525	-0.9030608736	10.2345885922
H27	0.0085251800	-1.1712161228	12.3300104216
H28	2.0030075371	0.2959443060	12.3310231095
H29	2.7321372172	1.4081293528	10.2091051796
H30	-1.2743920310	-1.5484425605	10.2408267481
C31	-0.7154085386	-0.4550926529	7.7179513727
H32	-1.5781319850	-1.1186671897	7.8250539957
P33	1.5236147457	1.2675168326	7.4407396233
S34	3.0605029067	2.4502857380	7.2488919269

7-H$^+$

E(M06-2X/6-311+G**) = -1471.64296549335

H(M06-2X/6-31+G*) = -1471.42370168184

C1	-2.4520367697	1.2750008902	6.9667105741
C2	-2.7568976263	2.5663933955	6.5266925780
C3	-1.7568832713	3.5192350982	6.3496463833
C4	-0.4255866171	3.1938719074	6.6114096132
C5	-0.1370688114	1.9070791979	7.0481357457
C6	1.4690740295	-0.2935468524	6.4532231366
C7	2.4312764731	-0.7082067510	5.5415694532
C8	2.2252904023	-1.9112465199	4.8650157634
C9	1.0768858187	-2.6610199377	5.1073449506
C10	0.1121523950	-2.2273347274	6.0216402238
C11	0.3005369522	-1.0341245257	6.7059159931
C12	-1.1336038535	0.9308569476	7.2331878348
H13	-3.2429452599	0.5422480554	7.0998057380
H14	-3.7896531070	2.8283390219	6.3202376713
H15	-2.0095064342	4.5171056180	6.0075819661

H16	0.3583177521	3.9336861831	6.4744240234
H17	3.3171664690	-0.1097597382	5.3468470730
H18	2.9608785498	-2.2583025138	4.1472790416
H19	0.9244142916	-3.5949805885	4.5760146185
H20	-0.7820416682	-2.8195143326	6.1949540573
C21	0.3210648909	-0.6878238217	11.4248175184
C22	1.4382174315	0.1435992955	11.4444953472
C23	1.8656765832	0.7690672927	10.2725628852
C24	1.1530396063	0.5336940140	9.1040167802
C25	0.0187893513	-0.2970015905	9.0663518499
C26	-0.3924614811	-0.9085862317	10.2429707459
H27	-0.0051681108	-1.1693813079	12.3410783883
H28	1.9766075656	0.3104187161	12.3713080946
H29	2.7275129800	1.4308658346	10.2823366624
H30	-1.2662326028	-1.5538552197	10.2445642070
C31	-0.6920316686	-0.4554890651	7.7188524564
H32	-1.5576522201	-1.1137245954	7.8210003659
P33	1.4575313522	1.1942956536	7.4609273247
S34	3.0267688612	2.5117543655	7.2365686962
H35	3.9439907627	1.6038125195	7.6274505276

7-Me$^+$

E(M06-2X/6-311+G**) = -1510.948912186
H(M06-2X/6-31+G*) = -1510.72242911044

C1	-2.4394065452	1.2721539612	6.9642428158
C2	-2.7361176777	2.5649165206	6.5218125585
C3	-1.7305406549	3.5118628720	6.3467192453
C4	-0.4015171777	3.1792540812	6.6129019687
C5	-0.1212932575	1.8914911899	7.0514165950

C6	1.4620506897	-0.3108160822	6.4495572968
C7	2.3904814882	-0.7052859369	5.4933041400
C8	2.1635784122	-1.8926190308	4.7966233285
C9	1.0231699736	-2.6486680067	5.0578260350
C10	0.0834046393	-2.2284620267	6.0028314315
C11	0.2944417212	-1.0499492049	6.7067107455
C12	-1.1237711290	0.9208352976	7.2346455505
H13	-3.2351005785	0.5442354023	7.0958321889
H14	-3.7668669036	2.8321441897	6.3120636763
H15	-1.9766278097	4.5108023239	6.0027694639
H16	0.3881552587	3.9131581482	6.4780724796
H17	3.2622078743	-0.0962548837	5.2704392299
H18	2.8746916573	-2.2215486565	4.0462633857
H19	0.8540215106	-3.5711401652	4.5116452336
H20	-0.8129698271	-2.8158516379	6.1811880970
C21	0.2653231092	-0.6591248895	11.4418337520
C22	1.3712294647	0.1875378833	11.4708075289
C23	1.8195448644	0.7924305948	10.2960899743
C24	1.1447366037	0.5203008738	9.1116581347
C25	0.0127021968	-0.3119126204	9.0706401447
C26	-0.4211322040	-0.9043652959	10.2495734148
H27	-0.0771944799	-1.1263435641	12.3595995704
H28	1.8823962026	0.3836024092	12.4073426674
H29	2.6621352497	1.4780213496	10.3187560967
H30	-1.2953558837	-1.5494100053	10.2448855148
C31	-0.6920649217	-0.4696001339	7.7218448938
H32	-1.5627497652	-1.1216257861	7.8216983461
P33	1.4757989258	1.1767914907	7.4664965936
S34	3.0557067394	2.4700863035	7.2517996479
C35	4.4373985210	1.3681603550	7.7595544306
H36	5.3284374048	1.9927296626	7.6767138724
H37	4.3227508172	1.0370402992	8.7907578038

H38	4.5307899512	0.5144505880	7.0898030709

7-F$^-$

E(M06-2X/6-311+G**) = -1571.19531232547

H(M06-2X/6-31+G*) = -1510.72242911044

C1	0.0086485471	-1.5762104451	6.3906475606
C2	-0.0060177845	-1.5547961221	4.9956586214
C3	0.2314759671	-0.3607116977	4.3148406943
C4	0.4978343344	0.8090074430	5.0267650228
C5	0.4971880744	0.7903848008	6.4176894454
C6	1.8677361803	1.4974455342	8.8159665116
C7	2.9891215152	2.0932079894	9.3844764016
C8	3.7016260373	1.4265207754	10.3814638228
C9	3.3083695896	0.1510762513	10.7868973816
C10	2.1927831937	-0.4524879639	10.2056713677
C11	1.4633396549	0.2209289659	9.2270883530
C12	0.2499880431	-0.4042324250	7.1059806769
H13	-0.1800619017	-2.5048492464	6.9265237992
H14	-0.2031448427	-2.4694858935	4.4419316873
H15	0.2236168518	-0.3442647946	3.2278140244
H16	0.7235222736	1.7406669566	4.5142775785
H17	3.3029454911	3.0703060847	9.0263347983
H18	4.5730809621	1.8951808814	10.8318151391
H19	3.8692483385	-0.3748866355	11.5556391842
H20	1.8803415898	-1.4463397379	10.5216126575
C21	-3.0151840013	1.2497302397	9.9941824993
C22	-2.8518778411	2.5480998538	9.5199469856
C23	-1.7222549676	2.8930415841	8.7686633272
C24	-0.7373415422	1.9512434224	8.4776337594

C25	-0.9215558710	0.6472940917	8.9668435027
C26	-2.0389947238	0.2905245568	9.7140331217
H27	-3.8929562619	0.9812668243	10.5776176376
H28	-3.6073288534	3.3013965604	9.7338670673
H29	-1.5931675681	3.9053561345	8.3967360810
H30	-2.1487917905	-0.7307775793	10.0768705835
C31	0.1847054560	-0.3395633909	8.6238717257
H32	-0.0277938537	-1.3317986629	9.0378293733
S33	0.6265807995	4.2199622636	7.0198644435
P34	0.9069151574	2.2729076700	7.4410550332
F35	2.4561182703	2.2533372070	6.5638091498

8

E(M06-2X/6-311+G**) = -3474.73553251064

H(M06-2X/6-31+G*) = -3474.54441872672

C1	-2.4601420079	1.2718332813	7.0031868879
C2	-2.7637137958	2.5634988989	6.5627818880
C3	-1.7563693467	3.5083888645	6.3841196647
C4	-0.4258978588	3.1713052263	6.6453254508
C5	-0.1332728643	1.8875008683	7.0823507837
C6	1.4559447911	-0.2718377154	6.4995806302
C7	2.4224904667	-0.6991682822	5.6007068905
C8	2.2272333819	-1.9048566409	4.9222258935
C9	1.0779673603	-2.6570106606	5.1523385029
C10	0.1088859724	-2.2192071308	6.0598921729
C11	0.2942734801	-1.0213209621	6.7393968184
C12	-1.1396800060	0.9271894648	7.2655687008
H13	-3.2520081488	0.5397006366	7.1402287847
H14	-3.7964153662	2.8300916601	6.3588808366

H15	-2.0041216566	4.5082046256	6.0418602253
H16	0.3778244042	3.8914331411	6.5130171318
H17	3.3111735677	-0.0944197863	5.4375737488
H18	2.9729300470	-2.2548315492	4.2154084663
H19	0.9304287800	-3.5935779829	4.6230303555
H20	-0.7857352286	-2.8117953259	6.2340292772
C21	0.3378013502	-0.6867541931	11.4425621656
C22	1.4592697605	0.1389413354	11.4458448094
C23	1.8728531035	0.7625750155	10.2659068472
C24	1.1490653758	0.5433105945	9.1027563584
C25	0.0174351862	-0.2861564833	9.0877275120
C26	-0.3859437339	-0.9020930011	10.2662144725
H27	0.0198607737	-1.1696261168	12.3616804141
H28	2.0134766786	0.2989096797	12.3652390392
H29	2.7448436543	1.4114106187	10.2430320197
H30	-1.2603342291	-1.5480587333	10.2715814806
C31	-0.6987222090	-0.4521568402	7.7498483790
H32	-1.5613717853	-1.1157817789	7.8556938748
P33	1.5409595440	1.2710465188	7.4732306426
Se34	3.1950252368	2.5436599169	7.2702682575

8-H$^+$

E(M06-2X/6-311+G**) = -3475.07915502396

H(M06-2X/6-31+G*) = -3474.88538530689

C1	-2.4395453324	1.2537627474	7.0025097054
C2	-2.7520389374	2.5432924606	6.5625225606
C3	-1.7569562852	3.5012647926	6.3843939128
C4	-0.4241623760	3.1818963851	6.6452694697
C5	-0.1270537799	1.8968612771	7.0815307539

C6	1.4893230349	-0.2947337125	6.4847998351
C7	2.4550938765	-0.7088746730	5.5767583265
C8	2.2554203543	-1.9147532852	4.9032669658
C9	1.1098465195	-2.6688768597	5.1459712994
C10	0.1424792599	-2.2367880663	6.0582296268
C11	0.3241957917	-1.0401204778	6.7390829751
C12	-1.1185671509	0.9159254540	7.2673405329
H13	-3.2260295879	0.5166558923	7.1372971064
H14	-3.7862716408	2.7995035255	6.3571612181
H15	-2.0148916852	4.4975656931	6.0423619099
H16	0.3548437522	3.9267240438	6.5077352879
H17	3.3399664764	-0.1081072945	5.3856867702
H18	2.9938792196	-2.2612539283	4.1885016966
H19	0.9619701221	-3.6051401750	4.6177280074
H20	-0.7487213742	-2.8326596375	6.2337502913
C21	0.3504998429	-0.6997365945	11.4548334467
C22	1.4649141404	0.1354103190	11.4729184965
C23	1.8866559330	0.7645201766	10.3009556720
C24	1.1717785828	0.5299793115	9.1338885912
C25	0.0408877512	-0.3052178669	9.0973891886
C26	-0.3650903070	-0.9209178299	10.2741969402
H27	0.0284268488	-1.1845795814	12.3706313561
H28	2.0056627457	0.3013137839	12.3982613898
H29	2.7472529600	1.4271322081	10.3069818315
H30	-1.2358606631	-1.5700870858	10.2761798392
C31	-0.6706495792	-0.4672331058	7.7517593549
H32	-1.5328669953	-1.1300017978	7.8541594642
P33	1.4807792400	1.1995152354	7.4904841430
Se34	3.1603308606	2.6092820356	7.2548765973
H35	4.1065971427	1.5615552239	7.6937900207

8-Me$^+$

E(M06-2X/6-311+G**) = -3514.39286190159

H(M06-2X/6-31+G*) = -3514.18482557093

C1	-2.4348408382	1.2564291188	6.9994509610
C2	-2.7430205970	2.5465774214	6.5571972920
C3	-1.7449843151	3.5014478399	6.3806253370
C4	-0.4130966671	3.1785141274	6.6450523534
C5	-0.1206290906	1.8932542685	7.0831098453
C6	1.4768167712	-0.2986514659	6.4817506485
C7	2.4114865971	-0.6921777970	5.5315393269
C8	2.1953583614	-1.8848044802	4.8397837776
C9	1.0591127615	-2.6473377234	5.1007444936
C10	0.1138657913	-2.2291589082	6.0415064309
C11	0.3145080714	-1.0453142071	6.7398656333
C12	-1.1157571583	0.9154356334	7.2679298587
H13	-3.2242085823	0.5220374628	7.1324805738
H14	-3.7761003262	2.8053578370	6.3489281596
H15	-1.9994108451	4.4982201111	6.0369396349
H16	0.3700098511	3.9191660200	6.5085639318
H17	3.2801081735	-0.0776094643	5.3113941706
H18	2.9112495888	-2.2129638226	4.0938479782
H19	0.8980062672	-3.5736637058	4.5588789327
H20	-0.7780110182	-2.8227229688	6.2214276357
C21	0.2977419834	-0.6630058697	11.4702961523
C22	1.3993504174	0.1894547589	11.4965552733
C23	1.8379376832	0.8010148617	10.3212804852
C24	1.1582232295	0.5302683688	9.1396060232
C25	0.0315856686	-0.3089799886	9.1011488338

C26	-0.3929115498	-0.9084042049	10.2802087260
H27	-0.0375449862	-1.1354135742	12.3879350956
H28	1.9143502455	0.3844833769	12.4310559271
H29	2.6777327725	1.4903393356	10.3393860217
H30	-1.2626142792	-1.5593908104	10.2772677666
C31	-0.6747325341	-0.4709481986	7.7544815422
H32	-1.5410954538	-1.1281134161	7.8553692310
P33	1.4899039264	1.1965024848	7.4943532584
Se34	3.1952263756	2.5657235325	7.2724820578
C35	4.5817747000	1.2842811631	7.8341107675
H36	5.5071153425	1.8595177938	7.7901876799
H37	4.4006663402	0.9473589812	8.8524555280
H38	4.6304495038	0.4464950802	7.1421130922

8-F^-

E(M06-2X/6-311+G**) = -3574.6388706846

H(M06-2X/6-31+G*) = -3574.4136923411

C1	-0.0379352328	-1.5808532698	6.3961589746
C2	-0.0514492462	-1.5583023134	5.0010373296
C3	0.1863929339	-0.3639421018	4.3205513204
C4	0.4522740985	0.8056370182	5.0328347275
C5	0.4501476453	0.7849020273	6.4237382409
C6	1.8207221325	1.4919586085	8.8197802317
C7	2.9429974178	2.0890537566	9.3848740889
C8	3.6567840548	1.4227493413	10.3812055656
C9	3.2634391137	0.1477584205	10.7884282314
C10	2.1466294530	-0.4563736623	10.2099410611
C11	1.4157295746	0.2164670472	9.2319254754

C12	0.2026125460	-0.4090476771	7.1121884741
H13	-0.2268801105	-2.5096579900	6.9311945852
H14	-0.2482856555	-2.4724179971	4.4466492828
H15	0.1787004032	-0.3468486567	3.2337501315
H16	0.6769068664	1.7380911087	4.5215265198
H17	3.2549503595	3.0664690732	9.0262651482
H18	4.5285834416	1.8917278975	10.8300361053
H19	3.8253168003	-0.3772965862	11.5567942038
H20	1.8346271397	-1.4496296550	10.5274339005
C21	-3.0645692985	1.2411380790	9.9989400099
C22	-2.9050561147	2.5401250357	9.5257842544
C23	-1.7763010891	2.8894726991	8.7749893282
C24	-0.7878928327	1.9516488440	8.4826266372
C25	-0.9684739578	0.6459073161	8.9708250966
C26	-2.0850184328	0.2857971258	9.7176024102
H27	-3.9412837492	0.9693394952	10.5820351014
H28	-3.6620869049	3.2914663581	9.7397242608
H29	-1.6531783494	3.9032578453	8.4059421476
H30	-2.1907221380	-0.7360420499	10.0788035370
C31	0.1365308528	-0.3424046431	8.6295355657
H32	-0.0784193395	-1.3333140724	9.0449198948
Se33	0.5871274888	4.3714127782	6.9762943207
P34	0.8578552921	2.2675428315	7.4471890577
F35	2.4072368200	2.2572027303	6.5652178407

9

E(M06-2X/6-311+G**) = -1947.3060782224

H(M06-2X/6-31+G*) = -1946.549463

E(BP86/6-31G*) = -1947.5464958065

C1	-2.3549672437	0.9057900430	6.2392233935
C2	-2.7022827116	2.1303494645	5.6608197578
C3	-1.7664514669	3.1544298419	5.5480066065
C4	-0.4607584757	2.9728306328	6.0118413877
C5	-0.1259143763	1.7518395179	6.5856766761
C6	1.7067590929	-0.2992382754	6.4044116056
C7	2.8302942349	-0.6829293607	5.6860339479
C8	2.8389905265	-1.9430915824	5.0841020940
C9	1.7362818169	-2.7849324047	5.2098986736
C10	0.6093266324	-2.3867734961	5.9351738442
C11	0.5894565461	-1.1356109685	6.5384762050
C12	-1.0620970774	0.7102447282	6.7066061376
H13	-3.0913318346	0.1105621249	6.3244172833
H14	-3.7145590512	2.2816428729	5.2977864616
H15	-2.0494890836	4.1017469808	5.0999756901
H16	0.2808262423	3.7649911140	5.9383272233
H17	3.6745828598	-0.0040170631	5.6038678625
H18	3.7063821262	-2.2658347465	4.5168527801
H19	1.7495425111	-3.7632926252	4.7388786583
H20	-0.2464171028	-3.0507404522	6.0267544486
C21	-0.0651959337	-0.4986643175	11.1611598920
C22	0.9615392295	0.4361609574	11.2599495825
C23	1.4855980115	1.0315544497	10.1102592261
C24	0.9638081541	0.6690477375	8.8744946576
C25	-0.0763550130	-0.2695025894	8.7632807907
C26	-0.5887111209	-0.8533488264	9.9147700217
H27	-0.4686842959	-0.9549187248	12.0602581188
H28	1.3532266599	0.7116384400	12.2341320348
H29	2.2643296495	1.7857075520	10.1682231347

H30	-1.3936411300	-1.5806250060	9.8445671481
C31	-0.5809910356	-0.5887710381	7.3556225723
H32	-1.3936136242	-1.3190434284	7.3975555525
P33	1.4981101802	1.2817050604	7.2482707558
N34	2.7945845047	2.1864817435	7.0568635733
S35	2.8883559109	3.7162476317	7.5910574151
O36	2.4454750169	3.8063906008	8.9883371390
O37	2.2851357593	4.6412068441	6.6279586447
C38	7.3985256064	4.4182106406	7.4897430495
C39	6.6037340542	4.7118838650	6.3746440645
C40	5.2292345219	4.5027746920	6.3978747392
C41	4.6457517819	3.9900780901	7.5529264293
C42	5.4068659933	3.6932059606	8.6760822225
C43	6.7826855682	3.9096458900	8.6362922669
H44	7.0695278246	5.1174241987	5.4793622264
H45	4.6042135363	4.7444478691	5.5438128456
H46	4.9221045363	3.3144052822	9.5706651173
H47	7.3852853596	3.6864640154	9.5129769870
C48	8.8859042823	4.6619028486	7.4452985263
H49	9.3624429930	4.3788803923	8.3872998242
H50	9.3539153795	4.0844133181	6.6409157934
H51	9.1035131085	5.7192859698	7.2598945288

9-H$^+$

E(M06-2X/6-311+G**) = -1947.6852806276

H(M06-2X/6-31+G*) = -1946.914724

C1	-2.3897936722	1.0685678681	6.9173647977
C2	-2.7859868779	2.2667259691	6.3163213868

C3	-1.8437466097	3.1893079262	5.8670276093
C4	-0.4805243742	2.9324613670	6.0160272713
C5	-0.1010169308	1.7372164113	6.6156794131
C6	1.5039896107	-0.4940680362	6.1647069651
C7	2.3679809193	-1.0458966601	5.2265657441
C8	2.1104050072	-2.3357042349	4.7604478542
C9	1.0101747914	-3.0435345357	5.2376336721
C10	0.1520714667	-2.4815649857	6.1870165086
C11	0.3914381850	-1.1984814391	6.6605759701
C12	-1.0375146755	0.7928723526	7.0703696462
H13	-3.1341599975	0.3563800449	7.2623063537
H14	-3.8437916583	2.4795906596	6.1987447755
H15	-2.1672403144	4.1152116858	5.4033511831
H16	0.2578565016	3.6530378720	5.6752019827
H17	3.2336797209	-0.5011182934	4.8596319449
H18	2.7710702148	-2.7848838364	4.0265618284
H19	0.8160441745	-4.0459539791	4.8698149663
H20	-0.7010668116	-3.0452135056	6.5538746985
C21	1.0237349890	-0.2054192115	11.2273082092
C22	2.1278378861	0.6066551513	10.9744909684
C23	2.3729792417	1.0710400463	9.6826722402
C24	1.4949312965	0.7021552850	8.6727352085
C25	0.3842687458	-0.1266230703	8.9054638948
C26	0.1533092620	-0.5770324853	10.1990648983
H27	0.8373502890	-0.5589013198	12.2363970935
H28	2.7973188085	0.8804896684	11.7830446362
H29	3.2292553166	1.7029566135	9.4677116077
H30	-0.6987925772	-1.2170621869	10.4086236002
C31	-0.4878050462	-0.4917275624	7.6988764443
H32	-1.3070867981	-1.1446696747	8.0070632082

P33	1.5562043278	1.1282163983	6.9361493505
S34	2.9669331545	3.7032413951	6.8367308158
O35	2.0281824385	3.7940862623	7.9400679781
O36	2.7833712537	4.4062932690	5.5859006827
C37	7.2070958482	4.3474272510	8.3100465623
C38	6.9283786606	4.2930374983	6.9354487117
C39	5.6355848167	4.0953804467	6.4720636243
C40	4.6129373723	3.9328863330	7.4083125619
C41	4.8482472788	3.9942108657	8.7791237344
C42	6.1525655776	4.2029597602	9.2178958982
H43	7.7366976026	4.4251856590	6.2212406925
H44	5.4172048334	4.0943808021	5.4080821293
H45	4.0233876145	3.9199235203	9.4813134604
H46	6.3510102440	4.2694379077	10.2835907766
C47	8.6156844073	4.5855487472	8.7829320950
H48	8.6882606246	4.5307636255	9.8709921734
H49	9.2995952209	3.8464081795	8.3544662686
H50	8.9628989740	5.5751553565	8.4681334946
N51	2.8770529302	2.0182910977	6.4336933682
H52	3.2426209935	1.8071788353	5.5043046053

9-Me$^+$

E(M06-2X/6-311+G**) = -1986.98035709831

H(M06-2X/6-31+G*) = -1986.170518

C1	-2.3905748727	1.0859421018	6.8567542433
C2	-2.7802664486	2.2763593428	6.2366439679
C3	-1.8336547033	3.1893712733	5.7753757081

C4	-0.4719138029	2.9284921494	5.9293643925
C5	-0.0986574109	1.7386439982	6.5448311697
C6	1.5437526073	-0.4985829220	6.1598289840
C7	2.4585120122	-1.1351291262	5.3252139459
C8	2.2223203267	-2.4564628080	4.9451344388
C9	1.0922932995	-3.1259257464	5.4034937491
C10	0.1958147845	-2.4942105108	6.2673371294
C11	0.4158087597	-1.1806574654	6.6598501109
C12	-1.0386907829	0.8096729168	7.0135553762
H13	-3.1380536932	0.3831901782	7.2140855790
H14	-3.8369268264	2.4926497096	6.1152178365
H15	-2.1537239463	4.1106499761	5.3003738262
H16	0.2713543654	3.6436067300	5.5850706323
H17	3.3532589143	-0.6328961390	4.9768394979
H18	2.9275721101	-2.9595566540	4.2921252386
H19	0.9116880898	-4.1520574798	5.0999506763
H20	-0.6708247508	-3.0304976039	6.6428106205
C21	1.0566649048	-0.1746786885	11.1780921639
C22	2.1788143905	0.6071009953	10.9132343967
C23	2.4167533299	1.0767839569	9.6223166674
C24	1.5171094127	0.7448363905	8.6187457316
C25	0.3963415922	-0.0686247376	8.8622713846
C26	0.1685665918	-0.5190765419	10.1567744812
H27	0.8734026283	-0.5292930636	12.1872759726
H28	2.8690683800	0.8552763981	11.7126631382
H29	3.2868363134	1.6864076103	9.4043216991
H30	-0.6945120151	-1.1436151715	10.3695689620
C31	-0.4808421324	-0.4526251197	7.6661189840
H32	-1.2922621874	-1.1082803845	7.9890646937
P33	1.5693234935	1.1664432711	6.8704830251

S34	2.9001871292	3.7500128080	6.9499382371
O35	2.0107677731	3.6836109827	8.0956420631
O36	2.6662091343	4.6469515665	5.8371476774
C37	7.2030032615	4.2258406600	8.3216609544
C38	6.8796541251	4.2657986345	6.9565742079
C39	5.5689253859	4.1226310963	6.5241710977
C40	4.5714056383	3.9130074884	7.4788940030
C41	4.8530980349	3.8849612621	8.8417415461
C42	6.1742694350	4.0435771567	9.2511782943
H43	7.6670639510	4.4318158093	6.2262181693
H44	5.3208701163	4.2027116085	5.4700771735
H45	4.0496144790	3.7829547188	9.5647176740
H46	6.4059362963	4.0404391337	10.3122501166
C47	8.6301637189	4.4091794569	8.7624263582
H48	8.7362921489	4.2802467912	9.8414402634
H49	9.2868697499	3.6898608545	8.2635590074
H50	8.9849342797	5.4121436824	8.5032633025
N51	2.7964936855	2.1473576258	6.2900872017
C52	3.2965185172	1.9812297527	4.9039818058
H53	3.3505659269	2.9671741981	4.4389179424
H54	4.2828315135	1.5124527291	4.9136344169
H55	2.5970486682	1.3856765438	4.3143199891

9-F^-

E(M06-2X/6-311+G**) = -2047.23567991735

H(M06-2X/6-31+G*) = -2046.447658

C1	0.3492053206	-1.4974761574	6.1363832490
C2	0.5563919029	-1.3174759493	4.7675984537

C3	0.8461978058	-0.0503555077	4.2622186278
C4	0.9459861525	1.0437340411	5.1231277729
C5	0.7202997557	0.8611723983	6.4845069159
C6	1.7021628332	1.3314420859	9.1095784950
C7	2.7253325171	1.8871793651	9.8713699943
C8	3.3218841601	1.1335336591	10.8826338800
C9	2.9162730047	-0.1823764218	11.1033377504
C10	1.9054808330	-0.7454618696	10.3227282905
C11	1.2864921473	0.0112302068	9.3300957525
C12	0.4189972055	-0.4067892458	7.0002944700
H13	0.1219757266	-2.4858304989	6.5314793362
H14	0.4910225427	-2.1696050011	4.0956312493
H15	1.0081503451	0.0850556586	3.1960394538
H16	1.2034794178	2.0367506927	4.7597465088
H17	3.0600852545	2.8993938863	9.6558398827
H18	4.1140484766	1.5677509384	11.4868541439
H19	3.3892570293	-0.7743661596	11.8827753795
H20	1.5907277300	-1.7733605221	10.4924740015
C21	-3.2999411825	0.8733134191	9.5103177092
C22	-3.1106253757	2.2173861309	9.1993810417
C23	-1.8920014008	2.6589482810	8.6726417062
C24	-0.8504950786	1.7593644059	8.4542296720
C25	-1.0569715808	0.4086401245	8.7704608157
C26	-2.2649365105	-0.0398011911	9.2929185277
H27	-4.2487564191	0.5324479222	9.9178027719
H28	-3.9160095423	2.9294229140	9.3643809770
H29	-1.7318254295	3.7030290810	8.4205545391
H30	-2.4008273521	-1.0943683178	9.5278405372
C31	0.1254432927	-0.5096290170	8.4924101367
H32	-0.1046042333	-1.5459591384	8.7641574443

N33	0.4721000635	3.7922183281	7.6270118106
S34	1.1643408362	4.8978506022	6.7015027001
O35	0.3674498795	6.1249339960	6.8347306853
O36	1.4569753797	4.4346381684	5.3349965057
C37	5.1928813746	6.0351417500	8.6106234346
C38	3.9817439603	6.4725654107	9.1608415060
C39	2.7660300138	6.1274279798	8.5779665938
C40	2.7534133278	5.3275941909	7.4370765533
C41	3.9411686153	4.8790965722	6.8758188484
C42	5.1540657803	5.2387860749	7.4638401154
H43	3.9941557293	7.0977394078	10.0523634897
P44	0.8716292876	2.2093238406	7.7217608581
F45	2.4884677444	2.4830972900	7.0912186887
H46	3.8981179877	4.2458462172	5.9958915537
H47	1.8235341895	6.4785643166	8.9885185402
H48	6.0863864044	4.8879732404	7.0257057189
C49	6.5046039379	6.4288333113	9.2459600168
H50	7.3491391728	5.9763535915	8.7179751185
H51	6.6417338981	7.5163527436	9.2304568278
H52	6.5507657284	6.1082479768	10.2929010260

9-He$_8$-ring complex at 1.7 Å

E(BP86/6-31G*) = -1970.6344634671

He1	2.0198000000	1.8633000000	11.4447000000
He2	6.2279999587	3.2546000007	9.1306998684
He3	4.8860000000	0.1785000000	10.2418000000
He4	3.3618000000	4.9395000000	10.3336000000

He5	3.1955000000	0.3896000000	11.1134000000
He6	5.0726000012	4.7343999277	9.5021000722
He7	6.1504000491	1.3674000138	9.4372000977
He8	2.0974000000	3.7505000000	11.1382000000
X9	4.1239000000	2.5590000000	10.2877000000
C10	-0.2766487412	-0.4089100388	5.4438438225
C11	0.4998163155	-0.4557701655	4.2755763117
C12	1.8001265414	0.0664719631	4.2816603691
C13	2.3191994584	0.6708237121	5.4384930222
C14	1.5383940883	0.7370237210	6.6001923641
C15	1.7449137835	-0.2940727443	9.0268376749
C16	2.7085346292	-1.2254326269	9.4402062915
C17	2.3332917730	-2.5194249252	9.8374816600
C18	0.9884571536	-2.9064661852	9.7983982643
C19	0.0340531487	-2.0232558022	9.2720228100
C20	0.4077472053	-0.7405632125	8.8476835369
C21	0.2410224418	0.1650137287	6.6129500111
H22	-1.2861737771	-0.8381928661	5.4559062054
H23	0.0908491203	-0.9103069144	3.3661896856
H24	2.4162389132	0.0219955205	3.3766144536
H25	3.3152356274	1.1177232864	5.4169663652
H26	3.7599320920	-0.9567424652	9.4545959803
H27	3.1038705681	-3.2220389282	10.1731395905
H28	0.6878996150	-3.9079838707	10.1259516776
H29	-1.0057282818	-2.3468546317	9.1408504758
C30	-2.0711382602	3.3941875712	9.1648243596
C31	-0.9100214122	4.1681781480	9.3159506067
C32	0.3540774736	3.6058415942	9.0808507074
C33	0.4397420940	2.2594002032	8.6968992836
C34	-0.7238795589	1.4911135245	8.5012791624

C35	-1.9823495867	2.0560823934	8.7484050960
H36	-3.0545603737	3.8392364754	9.3548912474
H37	-0.9854792800	5.2199790170	9.6128006067
H38	1.2585182870	4.2124203393	9.1711598161
H39	-2.8897350155	1.4578609172	8.5997043235
C40	-0.5129610704	0.0919060604	7.9551463439
H41	-1.4781256595	-0.4242105949	7.8195043973
P42	2.0164054980	1.4144325314	8.2971486828
N43	3.3659999910	2.3454000577	8.7809999617
S44	3.4887306657	3.5280980165	7.5121195688
O45	3.4071885577	4.9148154740	8.0269778970
O46	2.5310378544	3.2263442919	6.3969440332
C47	7.6176755643	3.0388689940	5.4800370986
C48	7.0374096521	4.3074883289	5.6831394070
C49	5.8092657815	4.4498431677	6.3419238240
C50	5.1424457413	3.3063335982	6.8063094848
C51	5.6951180918	2.0324568022	6.6161870324
C52	6.9245926723	1.9070725286	5.9551859997
H53	7.5581823277	5.2026885853	5.3208764202
H54	5.3655406552	5.4365348918	6.5060889803
H55	5.1816949790	1.1493659588	7.0090223803
H56	7.3593539110	0.9097969961	5.8129050247
C57	8.9618322720	2.9010374929	4.7966492642
H58	9.0964645520	1.8939582542	4.3659251303
H59	9.0801605173	3.6397809102	3.9844648710
H60	9.7914900417	3.0673968014	5.5105716491

9-He_8-ring complex at 2.2 Å

E(BP86/6-31G*) = -1970.6670953528

He1	2.0198000000	1.8633000000	11.4447000000
He2	6.2280000006	3.2546000002	9.1307000011
He3	4.8859999998	0.1785000016	10.2417999999
He4	3.3618000000	4.9395000000	10.3336000000
He5	3.1955000000	0.3896000000	11.1134000000
He6	5.0726000000	4.7344000000	9.5021000000
He7	6.1504000001	1.3673999991	9.4371999990
He8	2.0974000000	3.7505000000	11.1382000000
X9	4.1239000000	2.5590000000	10.2877000000
C10	-0.7944033970	-0.2544044766	5.2719190805
C11	-0.1563510883	-0.1995236838	4.0222492146
C12	1.1120469713	0.3848050874	3.9098006357
C13	1.7418851631	0.9429704302	5.0350568720
C14	1.0994460617	0.9037299877	6.2799812253
C15	1.5623296221	-0.1849927182	8.6934685176
C16	2.6028330458	-1.0164599914	9.1192931876
C17	2.3197201257	-2.3180703968	9.5661996101
C18	1.0002570135	-2.7894597933	9.5695980878
C19	-0.0356364804	-1.9833968205	9.0680573709
C20	0.2411792760	-0.6917825790	8.6032246005
C21	-0.1690266424	0.2791963961	6.4063487186
H22	-1.7796403005	-0.7266855463	5.3705274827
H23	-0.6503537258	-0.6211179039	3.1395015549
H24	1.6169588011	0.4224490549	2.9380678870
H25	2.7091621251	1.4380558607	4.9337816289
H26	3.6281589210	-0.6525255941	9.0920006650
H27	3.1368546217	-2.9630008668	9.9079818902
H28	0.7775590184	-3.8003476706	9.9293303844

H29	-1.0588074384	-2.3734636534	9.0054382877
C30	-2.2402392158	3.3643389097	9.3387992903
C31	-1.0796189331	4.1499037310	9.4167569022
C32	0.1593791460	3.6253651003	9.0145266801
C33	0.2107443328	2.3094889679	8.5354313681
C34	-0.9536182003	1.5210332283	8.4287096241
C35	-2.1830267844	2.0508537019	8.8416880706
H36	-3.2029353759	3.7798206775	9.6580518117
H37	-1.1371161660	5.1781905034	9.7900888188
H38	1.0703794191	4.2305568582	9.0590355932
H39	-3.0949629815	1.4458304648	8.7661975448
C40	-0.7772676660	0.1374789356	7.8147479664
H41	-1.7435056884	-0.3921914679	7.7607369445
P42	1.7338741911	1.4895328367	7.9445716303
N43	3.1441999994	2.2828999991	8.3401000000
S44	3.3695857883	3.5607167490	7.2418306691
O45	3.3816416227	4.8765189481	7.9236234374
O46	2.4208449742	3.4424172120	6.0854422971
C47	7.5081386392	2.9305549342	5.2782688903
C48	7.0373897260	4.2176076046	5.6112606621
C49	5.8067443343	4.3977771697	6.2544732938
C50	5.0277221638	3.2752056950	6.5733086596
C51	5.4733691161	1.9839762519	6.2599480776
C52	6.7068548418	1.8210779653	5.6136285555
H53	7.6465663616	5.0957029913	5.3627608509
H54	5.4445442726	5.3962945167	6.5177516278
H55	4.8679892033	1.1141134563	6.5345867717
H56	7.0576983539	0.8102682381	5.3707328362
C57	8.8494818750	2.7499525605	4.5991998952
H58	8.9693636430	1.7266768912	4.2045828046

H59	8.9753197827	3.4565438238	3.7591642375
H60	9.6825900748	2.9344483745	5.3038385958

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E(M06-2X/6-311+G**) = -1398.98093911486

H(M06-2X/6-31+G*) = -1398.283333

E(BP86/6-31G*) = -1399.1601949648

C1	-2.4026042967	1.3660033865	6.8641386016
C2	-2.6758942304	2.6734348257	6.4531220279
C3	-1.6521406224	3.6103350496	6.3340697085
C4	-0.3353128818	3.2511879409	6.6285354541
C5	-0.0730924771	1.9526778217	7.0441473261
C6	1.5206605112	-0.2068658502	6.4569699641
C7	2.5168030607	-0.6135198368	5.5794063866
C8	2.3405919623	-1.7999786221	4.8647358506
C9	1.1801464759	-2.5515710015	5.0329216477
C10	0.1788419490	-2.1313088067	5.9124693518
C11	0.3447320901	-0.9532620564	6.6303587740
C12	-1.0959022068	0.9986614726	7.1616947292
H13	-3.2063550381	0.6389990026	6.9502581617
H14	-3.6976783861	2.9584604579	6.2205448994
H15	-1.8761392827	4.6203343222	6.0053481407
H16	0.4785400205	3.9628092231	6.5224934646
H17	3.4060743725	-0.0040548379	5.4461381471
H18	3.1073734071	-2.1323951291	4.1720131104
H19	1.0477853817	-3.4723406966	4.4725846354
H20	-0.7258953584	-2.7215672586	6.0350121792

C21	0.2005628755	-0.7725896090	11.3391529486
C22	1.3291257723	0.0407928736	11.4121773867
C23	1.7935322566	0.6988602831	10.2709408527
C24	1.1097413488	0.5237440778	9.0753344774
C25	-0.0275719792	-0.2922135512	8.9901511729
C26	-0.4815544246	-0.9424933047	10.1307571096
H27	-0.1552929874	-1.2819946763	12.2298769190
H28	1.8489551651	0.1632894615	12.3573217832
H29	2.6710516983	1.3387206364	10.2983938054
H30	-1.3611344602	-1.5795392045	10.0827303951
C31	-0.6875236676	-0.4032785512	7.6163886794
H32	-1.5605774663	-1.0600347016	7.6622878155
P33	1.5545094449	1.2827077213	7.4971821588
N34	2.8585157155	2.2012825995	7.6435927965
C35	3.2832857643	2.8202334576	6.4953105230
O36	2.7232581812	2.7105648937	5.4009101634
C37	4.5413045338	3.6808142282	6.6735434531
C38	5.6828680628	2.7803088275	7.1681069543
H39	6.5956639693	3.3739987491	7.2960803576
H40	5.4264486980	2.3169892984	8.1247367535
H41	5.8962670268	1.9839925143	6.4453498671
C42	4.2526033603	4.7620511403	7.7250792028
H43	5.1388584414	5.3927377174	7.8628342914
H44	3.4246714753	5.4070728041	7.4082103666
H45	3.9883732826	4.3104418758	8.6850159711
C46	4.9204203704	4.3281978773	5.3426494576
H47	5.8189133327	4.9426191901	5.4729937737
H48	5.1212608050	3.5710739821	4.5789842255
H49	4.1124132787	4.9640234502	4.9691105710

10-H$^+$

E(M06-2X/6-311+G**) = -1399.372196782

H(M06-2X/6-31+G*) = -1398.658159

C1	-2.3222603042	1.4506147754	6.7867620300
C2	-2.5574088124	2.7771046369	6.4153064630
C3	-1.5227670777	3.7097849698	6.3897822276
C4	-0.2268528467	3.3287824531	6.7372940013
C5	-0.0080120318	2.0089239908	7.1105864950
C6	1.6064633014	-0.1895084935	6.5106761466
C7	2.6442501003	-0.5813428477	5.6747907537
C8	2.4763742783	-1.7370191720	4.9121114122
C9	1.2906974383	-2.4640084655	4.9941210559
C10	0.2522301799	-2.0555950565	5.8354245042
C11	0.4026768122	-0.9093058945	6.6045515760
C12	-1.0390398703	1.0537778515	7.1392746404
H13	-3.1377116815	0.7329549584	6.7990139795
H14	-3.5615697121	3.0826062008	6.1391295904
H15	-1.7217545852	4.7338142830	6.0922552893
H16	0.5909748278	4.0422111968	6.7028073519
H17	3.5564234218	0.0035526525	5.6050309225
H18	3.2699392510	-2.0646969847	4.2490398988
H19	1.1683631496	-3.3598757914	4.3937769978
H20	-0.6680095556	-2.6305382533	5.8878337296
C21	0.0102609017	-0.9010830236	11.3117545981
C22	1.1463646405	-0.1152968601	11.4881671556
C23	1.6892651712	0.5798108365	10.4072553220
C24	1.0737264372	0.4681587620	9.1652778894

C25	-0.0742721730	-0.3221530905	8.9739114786
C26	-0.6019399748	-1.0072384932	10.0602418490
H27	-0.4065101669	-1.4391266692	12.1570737382
H28	1.6119465685	-0.0416440762	12.4650971850
H29	2.5762368940	1.1905790991	10.5534068383
H30	-1.4877509470	-1.6235224811	9.9357145709
C31	-0.6663879480	-0.3714083961	7.5620496861
H32	-1.5486261263	-1.0147806968	7.5449344799
P33	1.5285451601	1.2291111754	7.6032745326
C34	3.3851965911	2.8594101193	6.6140468505
O35	2.7886786428	2.7055337360	5.5726012651
C36	4.6272949870	3.7100450230	6.8255644167
C37	5.7752855380	2.8078553089	7.3129965548
H38	6.6862418528	3.4070846397	7.4020376625
H39	5.5797944455	2.3656245218	8.2964811362
H40	5.9742318147	1.9976451772	6.6039305372
C41	4.3194759579	4.7973592969	7.8705903166
H42	5.1905177522	5.4515337842	7.9713000902
H43	3.4689393715	5.4153728013	7.5649172196
H44	4.1072172819	4.3847720597	8.8634746494
C45	4.9964746707	4.3548446972	5.4879117988
H46	5.8907344341	4.9708401773	5.6197522360
H47	5.2042076889	3.5981881198	4.7267362217
H48	4.1878603405	4.9902669970	5.1170608622
N49	2.8858515063	2.1843733032	7.7536779774
H50	3.3450159508	2.2799796235	8.6540092684

10-Me$^+$

E(M06-2X/6-311+G**) = -1438.65663479280

H(M06-2X/6-31+G*) = -1437.903327

C1	-2.2987481989	1.6522197320	6.9568159216
C2	-2.4867831257	3.0207710084	6.7459363199
C3	-1.4194808908	3.9143663682	6.8241310545
C4	-0.1381223081	3.4484540855	7.1165430957
C5	0.0331633732	2.0868002732	7.3332743123
C6	1.6088843580	-0.0743832164	6.4807103747
C7	2.6390858616	-0.4427014588	5.6241462249
C8	2.4329894425	-1.5160688763	4.7583609361
C9	1.2126391758	-2.1872159226	4.7511206468
C10	0.1831003349	-1.8071175300	5.6143547058
C11	0.3741453515	-0.7488084639	6.4939460316
C12	-1.0285964335	1.1749495985	7.2546574150
H13	-3.1385605075	0.9666694669	6.8862465410
H14	-3.4795890603	3.3922387600	6.5125866416
H15	-1.5832889246	4.9723861225	6.6489730698
H16	0.7068355351	4.1313887821	7.1592336727
H17	3.5784509232	0.0996353541	5.6140026421
H18	3.2250602683	-1.8197379475	4.0821122512
H19	1.0577824021	-3.0157157381	4.0673662761
H20	-0.7645982947	-2.3382275730	5.6031884744
C21	0.0429404859	-1.4234335232	11.0962058418
C22	1.2330138417	-0.7474955395	11.3490926203
C23	1.7761353622	0.1031582716	10.3857571122
C24	1.1064972726	0.2716222927	9.1758024669
C25	-0.0791472211	-0.4374325537	8.8994155096
C26	-0.6083275847	-1.2779754367	9.8699601944
H27	-0.3758242304	-2.0809633397	11.8513037952

H28	1.7462846786	-0.8827435354	12.2952638623
H29	2.7142711470	0.6062200163	10.5895106958
H30	-1.5225659079	-1.8287463687	9.6672542424
C31	-0.6864378470	-0.2927496335	7.5030122156
H32	-1.5799817211	-0.9144370660	7.4145569632
P33	1.5647003591	1.2373705584	7.7148453323
C34	3.4023194107	2.7876828201	6.7477654627
O35	2.7618069798	2.5404867464	5.7449485055
C36	4.6906505259	3.6144988837	6.7170487541
C37	5.7108226402	3.2283736777	7.7996686133
H38	6.6920402813	3.6095663336	7.5022464614
H39	5.4912619189	3.6594269551	8.7782309162
H40	5.8009208418	2.1411576501	7.9045424318
C41	4.3032790307	5.1035151124	6.8175574225
H42	5.2090453017	5.7105451406	6.7223803746
H43	3.6197678104	5.3811153809	6.0094720676
H44	3.8356841958	5.3620614168	7.7733639474
C45	5.3218849358	3.3651813231	5.3357043902
H46	6.2074637084	3.9985719301	5.2317079273
H47	5.6363462200	2.3212859301	5.2296793234
H48	4.6240866140	3.5976020385	4.5299054475
N49	2.9017785822	2.2372827608	7.9592928868
C50	3.1096926836	2.8460584487	9.2912475979
H51	3.3311078481	3.9051190231	9.1707725801
H52	2.1896695014	2.7705704569	9.8749728265
H53	3.9267650602	2.3596953934	9.8262616131

10-F^-

E(M06-2X/6-311+G**) = -1498.894430795

H(M06-2X/6-31+G*) = -1498.165083

C1	0.2711742204	-1.6529060578	6.4374068090
C2	0.2554410770	-1.6175174112	5.0429135628
C3	0.2789418396	-0.3925335128	4.3763043307
C4	0.3366317447	0.8014332635	5.0961097857
C5	0.3416364379	0.7625005292	6.4882694564
C6	1.6215921149	1.6343519240	8.8787860464
C7	2.6503315233	2.3917811248	9.4296077129
C8	3.4784123978	1.8333654342	10.4035757990
C9	3.2921478371	0.5098212395	10.8016630130
C10	2.2687346240	-0.2534271318	10.2377249723
C11	1.4225355606	0.3076160037	9.2832107094
C12	0.3024369972	-0.4646763003	7.1654330723
H13	0.2481912881	-2.6054143976	6.9633985244
H14	0.2221731355	-2.5464491391	4.4787113594
H15	0.2627568110	-0.3660141481	3.2896080061
H16	0.3681732503	1.7716331269	4.6072731890
H17	2.8009493900	3.4092158819	9.0793745634
H18	4.2776390519	2.4256952544	10.8416613022
H19	3.9442130887	0.0694835854	11.5519105577
H20	2.1211413557	-1.2861429111	10.5480818312
C21	-3.1770333227	0.6177005701	10.0705282735
C22	-3.2136291301	1.9323150771	9.6125433199
C23	-2.1429978119	2.4561366670	8.8783753518
C24	-1.0280993660	1.6732609045	8.5889530337
C25	-1.0106441222	0.3506754785	9.0556149288
C26	-2.0645055581	-0.1810198613	9.7899390246
H27	-4.0079092629	0.2121991454	10.6430174202

H28	-4.0780056636	2.5563490796	9.8289683618
H29	-2.1602881133	3.4845251684	8.5270576308
H30	-2.0228660260	-1.2114728485	10.1402308699
C31	0.2376380121	-0.4387264798	8.6868268509
H32	0.1938953347	-1.4595938237	9.0824969252
N33	0.0534897922	3.8401168590	7.5382749800
P34	0.5133870052	2.2581648014	7.5578726587
F35	1.9513232360	2.6249017677	6.6307061629
C36	-0.2418919292	4.4304648246	6.3823034012
O37	-0.3893710847	3.8873688394	5.2663366781
C38	-0.4582087184	5.9639590576	6.4556578874
C39	-1.8745159156	6.2661187465	5.9509461118
H40	-2.0486044557	7.3506409060	5.9161140371
H41	-2.0134830129	5.8476400779	4.9500856047
H42	-2.6264217366	5.8205601579	6.6144568988
C43	-0.2796568467	6.5229952675	7.8668738722
H44	-0.4358965308	7.6114009973	7.8615509981
H45	-0.9905795134	6.0686645509	8.5644993815
H46	0.7246720555	6.3115339226	8.2461875917
C47	0.5644289210	6.6096349863	5.5111806190
H48	0.4343219444	7.7007951534	5.4925420529
H49	1.5865033523	6.3883765493	5.8407257770
H50	0.4421143877	6.2160330035	4.4981116141

10-He$_8$-ring complex at 1.7 Å

E(BP86/6-31G*) = -1422.2361642597

He1	2.0197999952	1.8632999973	11.4447000195

He2	6.2279998128	3.2546000475	9.1306999956
He3	4.8859999874	0.1785000004	10.2417999808
He4	3.3618000466	4.9395000164	10.3336000049
He5	3.1955000060	0.3896000013	11.1134000113
He6	5.0726001167	4.7343999719	9.5021000294
He7	6.1504000476	1.3674000254	9.4372000064
He8	2.0973999787	3.7504999936	11.1381999551
X9	4.1239000000	2.5590000000	10.2877000000
C10	-0.2777530067	-0.8057800520	5.8348235087
C11	-0.4543617251	0.0287267043	4.7176765880
C12	0.1404350060	1.2939720878	4.7057005941
C13	0.9292914572	1.7221491406	5.7903406641
C14	1.1486924827	0.8816653282	6.8852023196
C15	3.0035402294	-0.4421738037	8.3432799265
C16	4.3706774332	-0.5904283893	8.0706853530
C17	4.9053244073	-1.8721894680	7.8692228302
C18	4.0732639242	-3.0005335914	7.9243961308
C19	2.6902826016	-2.8457659039	8.1098225055
C20	2.1496094009	-1.5641047189	8.2855534558
C21	0.5079569477	-0.3911549220	6.9162511767
H22	-0.7639269343	-1.7885257758	5.8723966396
H23	-1.0687305147	-0.3066778331	3.8747416950
H24	-0.0114596741	1.9692238063	3.8560256514
H25	1.3462069564	2.7241981999	5.7846277938
H26	5.0030540573	0.2974810228	8.0197782563
H27	5.9755541555	-1.9877275852	7.6642123570
H28	4.4947469107	-4.0021177754	7.7811361589
H29	2.0248626257	-3.7171798871	8.0752931308
C30	-1.6908435255	0.1206568900	10.8661715179
C31	-1.1976149580	1.4306286656	10.9650415049

C32	-0.0276014009	1.7977945267	10.2826626628
C33	0.6650821689	0.8438757430	9.5218598243
C34	0.1053603811	-0.4393106027	9.3267504160
C35	-1.0547758275	-0.8056657217	10.0252444788
H36	-2.5983564109	-0.1691471396	11.4080773526
H37	-1.7296276318	2.1763654406	11.5659981425
H38	0.3422150493	2.8234602835	10.3234938373
H39	-1.4834884303	-1.8046062959	9.8768780577
C40	0.6628200854	-1.2696717046	8.1759850217
H41	0.0876608535	-2.2043031045	8.0609703058
P42	2.1595329057	1.1877736340	8.4648537101
N43	3.3660000089	2.3453999462	8.7809999971
C44	2.8166185563	3.4774528592	8.1226330773
O45	1.5754791887	3.6886892161	8.1224047969
C46	3.6515894118	4.4784799287	7.2068145274
C47	2.9665808481	4.4338543513	5.8074992693
H48	3.4185283758	5.2133451414	5.1677512686
H49	3.1329858749	3.4650481244	5.3043677639
H50	1.8864797923	4.6349644221	5.8880870704
C51	5.1363489486	4.1329780685	6.9433615102
H52	5.4285661283	4.5187869075	5.9495001102
H53	5.8272643881	4.5805613599	7.6665578557
H54	5.2938397734	3.0417722459	6.9408088067
C55	3.4645073650	5.9403153730	7.6952926948
H56	3.8503779147	6.6326668728	6.9241814186
H57	2.3914058710	6.1503376283	7.8412667199
H58	3.9915132089	6.1658136760	8.6319718065

10-He$_8$-ring complex at 2.2 Å

E(BP86/6-31G*) = -1422.269041653

He1	2.0198000000	1.8633000000	11.4447000000
He2	6.2280000074	3.2546000010	9.1306999956
He3	4.8860000000	0.1785000000	10.2418000000
He4	3.3618000000	4.9395000000	10.3336000000
He5	3.1955000000	0.3896000000	11.1134000000
He6	5.0725999955	4.7343999960	9.5021000017
He7	6.1503999989	1.3674000006	9.4372000033
He8	2.0974000000	3.7505000000	11.1382000000
X9	4.1239000000	2.5590000000	10.2877000000
C10	0.0347255096	-1.2379137661	5.3864612581
C11	-0.1375933385	-0.4264116173	4.2525156794
C12	0.3589040971	0.8817096857	4.2498509862
C13	1.0419044309	1.3849390733	5.3714363827
C14	1.2408672232	0.5727266920	6.4918659797
C15	3.1401039645	-0.5381127243	8.0955206698
C16	4.5376366749	-0.5497297043	8.0113652332
C17	5.2128078052	-1.7761865832	7.9053253415
C18	4.4899474665	-2.9782023816	7.8706430986
C19	3.0855672202	-2.9611645655	7.8922968604
C20	2.4067531561	-1.7385609738	7.9810464286
C21	0.7150809375	-0.7485376484	6.5066450619
H22	-0.3673752625	-2.2585022689	5.4015930700
H23	-0.6712307906	-0.8171253071	3.3787580861
H24	0.2097414751	1.5267819229	3.3766791910
H25	1.3906334725	2.4156783162	5.3760397879
H26	5.0769658511	0.3986889116	8.0238275401
H27	6.3068748836	-1.7917334419	7.8448969284

H28	5.0201289866	-3.9346462287	7.7962483841
H29	2.5187854992	-3.8966460310	7.8105378011
C30	-1.6089946183	-0.4417070998	10.4527324351
C31	-1.2301882032	0.9023774556	10.5846568443
C32	-0.0989427557	1.3879057901	9.9103272436
C33	0.6627075089	0.5136051655	9.1241943236
C34	0.2286373973	-0.8163703282	8.9102153224
C35	-0.8943951794	-1.2959789159	9.5976967493
H36	-2.4886361955	-0.8194458710	10.9864727860
H37	-1.8241670350	1.5828809769	11.2048105516
H38	0.1768500704	2.4427911255	9.9638459779
H39	-1.2313267334	-2.3278383613	9.4386087476
C40	0.9028861743	-1.5942026415	7.7818217396
H41	0.4291704411	-2.5824590490	7.6578274659
P42	2.1253659551	0.9858112337	8.0938232908
N43	3.1443999983	2.2829000024	8.3402999995
C44	2.4830261614	3.3825782351	7.7540959813
O45	1.2339668576	3.4956980124	7.7573259549
C46	3.2821222370	4.4608447783	6.9243171941
C47	2.6182585940	4.5249128066	5.5203071546
H48	3.0541266517	5.3646440610	4.9483402385
H49	2.8144970288	3.6062785340	4.9395376252
H50	1.5302275282	4.6800736656	5.6049522707
C51	4.7612159957	4.1131289739	6.6886384805
H52	5.2377901915	4.9036816612	6.0777347614
H53	5.3249925722	4.0072107262	7.6167792997
H54	4.8530063349	3.1604638535	6.1377751528
C55	3.0943521495	5.8758591374	7.5309523164
H56	3.4471890215	6.6351801129	6.8083471576
H57	2.0253081064	6.0605440468	7.7329321614

H58	3.6556405604	6.0253917597	8.4603426152

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E(M06-2X/6-311+G**) = -2158.15026310439

H(M06-2X/6-31+G*) = -2157.254952

E(BP86/6-31G*) = -2158.387955147

C1	-2.8752171347	0.3498195655	7.4354549250
C2	-3.5265824825	1.2759169705	6.6152580058
C3	-2.7975681323	2.1703237226	5.8364283934
C4	-1.4003977028	2.1499883443	5.8577036250
C5	-0.7624329558	1.2165583598	6.6660009117
C6	1.1045819198	-0.8081709462	6.6025175574
C7	1.9496776563	-1.4673510805	5.7209568526
C8	1.8906369503	-2.8611747676	5.6519599428
C9	0.9961002638	-3.5620387103	6.4576667680
C10	0.1472195331	-2.8878362238	7.3409966894
C11	0.1978839716	-1.5016244903	7.4173551283
C12	-1.4873252816	0.3165123825	7.4664388841
H13	-3.4505556879	-0.3405879721	8.0473406723
H14	-4.6121440647	1.2994249747	6.5925922312
H15	-3.3137290270	2.8940561095	5.2134100868
H16	-0.8158667854	2.8650510782	5.2853748981
H17	2.6349697374	-0.8961231760	5.1003108045
H18	2.5415656442	-3.3979821214	4.9688485161
H19	0.9547873393	-4.6457064209	6.3994239383
H20	-0.5489446030	-3.4446007097	7.9631593299
C21	1.0508245725	0.8853662363	11.4049519439

C22	1.9539341936	1.7449450044	10.7840079148
C23	2.0041112319	1.8224190782	9.3893962490
C24	1.1366563464	1.0297018429	8.6488547036
C25	0.2205275036	0.1607297960	9.2627317874
C26	0.1825640415	0.0905018440	10.6492837375
H27	1.0173155722	0.8305448335	12.4890382881
H28	2.6198554881	2.3582724752	11.3829760444
H29	2.7012263438	2.4884075209	8.8857131139
H30	-0.5193404393	-0.5765059651	11.1436662968
C31	-0.6834459954	-0.6537498752	8.3349976234
H32	-1.3549084507	-1.2910960379	8.9168324488
P33	1.0302835011	0.9803511379	6.8395394550
N34	2.0891635611	1.7501905500	5.9603648639
P35	2.2443846579	3.3456434926	5.7649501228
O36	1.0379443968	4.2001345882	5.8214700966
O37	3.0198898212	3.5733611996	4.3603764976
O38	3.3962622076	3.7350748127	6.8593480932
C39	7.0961633398	3.0241813375	3.7466035765
C40	6.4477647412	4.1758031975	3.2989742500
C41	5.0829826409	4.3403385919	3.5107251218
C42	4.3708398522	3.3429273112	4.1709866495
C43	4.9959737494	2.1810902116	4.6141540976
C44	6.3660517884	2.0327503743	4.3995307717
H45	8.1628403536	2.9006228837	3.5862558796
H46	7.0083953609	4.9569661247	2.7942016930
H47	4.5586096978	5.2383376417	3.1991350903
H48	4.4165838310	1.4237720284	5.1327374794
H49	6.8636649299	1.1324106828	4.7487266387
C50	5.6434849633	7.2245087247	6.5761788688
C51	6.2498409241	6.0002483222	6.8604584422

C52	5.4839213358	4.8423267771	6.9501186493
C53	4.1070787193	4.9228048888	6.7602605586
C54	3.4800786055	6.1346211195	6.4846288673
C55	4.2637543978	7.2844718479	6.3900953377
H56	6.2436333032	8.1261232010	6.5001766679
H57	7.3253569176	5.9422447964	6.9994155682
H58	5.9335567847	3.8716475081	7.1370025326
H59	2.4046631596	6.1627543201	6.3379140630
H60	3.7853334394	8.2345996883	6.1709372351

11-H$^+$

E(M06-2X/6-311+G**) = -2158.527111195

H(M06-2X/6-31+G*) = -2157.619910

C1	-2.7927599750	0.5632806479	6.6647487119
C2	-3.1122906860	1.3803480408	5.5769169056
C3	-2.1184190859	2.0515630239	4.8676953007
C4	-0.7802306002	1.9186320440	5.2375267193
C5	-0.4771585936	1.0994459744	6.3173649575
C6	1.1246941070	-1.0623185423	7.0240562141
C7	2.0603892197	-1.9407854222	6.4907950205
C8	1.8383629556	-3.3122995060	6.6166937602
C9	0.6962067217	-3.7768128106	7.2636833134
C10	-0.2411888152	-2.8861316832	7.7932753104
C11	-0.0346945157	-1.5178152415	7.6781929796
C12	-1.4655473808	0.4149611072	7.0454561834
H13	-3.5770390257	0.0470929820	7.2108391736
H14	-4.1510901953	1.4944124325	5.2836946149

H15	-2.3837809165	2.6868511645	4.0293567800
H16	-0.0005185367	2.4538075046	4.7034641284
H17	2.9509701450	-1.5852428819	5.9792029563
H18	2.5570151046	-4.0145144686	6.2078432251
H19	0.5294658329	-4.8451126921	7.3573367633
H20	-1.1297277039	-3.2615261772	8.2930596169
C21	0.1418325923	1.3983169579	11.3897943990
C22	1.2647376137	2.0691284471	10.9089724246
C23	1.6478456956	1.9284788178	9.5750207238
C24	0.8860417473	1.1037534181	8.7572940544
C25	-0.2489832389	0.4197701407	9.2242628199
C26	-0.6178979111	0.5744008255	10.5542997984
H27	-0.1506748552	1.5178661028	12.4281977800
H28	1.8405206683	2.7079740758	11.5702404086
H29	2.5118026657	2.4589976841	9.1848232179
H30	-1.4921321821	0.0586884029	10.9417344481
C31	-1.0005839756	-0.4579887290	8.2172642769
H32	-1.8572491734	-0.9376418541	8.6956511417
P33	1.1291049514	0.7337717014	7.0208149823
P34	2.6599606672	3.0408111748	6.1356452118
O35	1.4792944036	3.6505683147	6.7621967232
O36	2.8266574972	3.3650414650	4.5875811385
O37	4.0958830291	3.2104538952	6.8030420655
C38	6.4014005830	4.3045205270	2.6721315943
C39	5.4714261561	5.3042061494	2.9603829201
C40	4.2747322845	4.9885674415	3.5970096378
C41	4.0368451859	3.6648711248	3.9384179801
C42	4.9332680311	2.6490233792	3.6449293056
C43	6.1292528041	2.9797388592	3.0076164930
H44	7.3333751411	4.5569918100	2.1768806192

H45	5.6790526426	6.3357527181	2.6947223710
H46	3.5409023803	5.7482068038	3.8474993666
H47	4.6986571659	1.6187732139	3.8979696959
H48	6.8438465196	2.1982491537	2.7694618789
C49	6.1510270120	6.8337791131	6.7132154104
C50	6.8032282384	5.6366839864	6.4139927997
C51	6.1095886023	4.4312043486	6.4498505114
C52	4.7653947762	4.4549288721	6.7917605238
C53	4.0921085349	5.6249884988	7.1150644234
C54	4.8036227968	6.8246576265	7.0652725096
H55	6.6961450691	7.7715176880	6.6798901982
H56	7.8543304732	5.6402724422	6.1434409003
H57	6.5856389368	3.4886175668	6.1994549003
H58	3.0428111222	5.6024994481	7.3952817671
H59	4.2968874814	7.7524798994	7.3110444702
N60	2.4676445460	1.3569683013	6.2600342250
H61	3.2201745071	0.7235799935	6.0007663582

11-Me$^+$

E(M06-2X/6-311+G**) = -2197.823050155

H(M06-2X/6-31+G*) = -2196.875436

C1	-2.6834786672	1.0275143375	6.4132013932
C2	-2.8240148205	1.6828103871	5.1870804652
C3	-1.7085369334	2.0227579736	4.4238909716
C4	-0.4265724894	1.7182966536	4.8804240784
C5	-0.3009029885	1.0662831536	6.1008225295
C6	0.8627139565	-1.2133882983	7.1913662535

C7	1.5794340477	-2.3549708190	6.8383637640
C8	1.0635836680	-3.6098006086	7.1630428712
C9	-0.1525033265	-3.7185014116	7.8284724440
C10	-0.8735730485	-2.5742876266	8.1729005480
C11	-0.3779821989	-1.3158081827	7.8580512315
C12	-1.4136706611	0.7112908134	6.8792529577
H13	-3.5604987224	0.7648513190	6.9980923367
H14	-3.8172013803	1.9292599004	4.8253389590
H15	-1.8341583877	2.5324131332	3.4745487275
H16	0.4484321421	1.9956443879	4.2997408031
H17	2.5239345828	-2.2962080090	6.3139681880
H18	1.6188403323	-4.5009939701	6.8903313500
H19	-0.5475967680	-4.6978443846	8.0783653423
H20	-1.8270586587	-2.6634704542	8.6857266549
C21	0.2884382987	2.0338899607	11.1074817119
C22	1.5334928228	2.3845245165	10.5874377548
C23	1.9003229258	1.9695630354	9.3073858357
C24	0.9972835255	1.2018044334	8.5818145964
C25	-0.2568103607	0.8361734339	9.0919049739
C26	-0.6092714411	1.2600331900	10.3670102827
H27	0.0108709566	2.3646136295	12.1032628507
H28	2.2195156901	2.9837263322	11.1769123875
H29	2.8668449709	2.2421847329	8.8908501996
H30	-1.5752538779	0.9909164690	10.7849581071
C31	-1.1387744756	-0.0290189992	8.1906158183
H32	-2.0773112816	-0.2710920548	8.6938634148
P33	1.2070697734	0.5459830458	6.9249800272
P34	2.9423758855	2.5822418953	5.9098262750
O35	1.7941194650	3.3984513521	6.3306971842
O36	3.3226299870	2.5683629345	4.3581919058

O37	4.3193283993	2.7872561817	6.6956417277
C38	5.7603913318	5.5861538400	2.8406768931
C39	4.5714255151	5.9250512218	3.4856341519
C40	3.7292136345	4.9314774877	3.9810123337
C41	4.1190591552	3.6066084661	3.8328060078
C42	5.2893415481	3.2403572017	3.1858263607
C43	6.1121359048	4.2463465987	2.6821884025
H44	6.4086775461	6.3660090596	2.4544573131
H45	4.2923852324	6.9670399464	3.6049255412
H46	2.7989319569	5.1767463268	4.4864394113
H47	5.5431047498	2.1896332547	3.0836948558
H48	7.0308184557	3.9801111339	2.1691280231
C49	6.0670420077	6.5296156399	7.2702384731
C50	6.7652467578	5.5133221677	6.6178352213
C51	6.1758455220	4.2665452679	6.4271330127
C52	4.8867664522	4.0661399345	6.8987342636
C53	4.1710648942	5.0522309142	7.5635904083
C54	4.7771077786	6.2959777167	7.7421144643
H55	6.5297459061	7.5006912514	7.4134245150
H56	7.7708143394	5.6902630699	6.2496551807
H57	6.6921347478	3.4644161353	5.9096865714
H58	3.1592326759	4.8603001109	7.9066591731
H59	4.2327954014	7.0833027912	8.2539273445
N60	2.6444653132	0.9378970584	6.1747391386
C61	3.6953986839	-0.0517168405	5.8412588612
H62	4.5830525000	0.4972448945	5.5258698551
H63	3.9588753169	-0.6410261369	6.7212868258
H64	3.3703919257	-0.6902752456	5.0181826826

11-F^-

E(M06-2X/6-311+G**) = -2258.075823555

H(M06-2X/6-31+G*) = -2257.14976

C1	-2.6955926338	-1.4216594361	6.9191603565
C2	-3.6976810911	-0.8883934303	6.1034875208
C3	-3.5407518975	0.3845032575	5.5609756960
C4	-2.3862049008	1.1294712059	5.8276356297
C5	-1.3779627593	0.6098443639	6.6363326028
C6	1.2261441520	0.0389639918	6.5836191946
C7	2.3234260065	0.0926522980	5.7300917116
C8	3.0224810005	-1.0770175430	5.4298889639
C9	2.6424997186	-2.2859916157	6.0113340786
C10	1.5553844650	-2.3333787565	6.8855313437
C11	0.8356554202	-1.1744464125	7.1675905884
C12	-1.5528819406	-0.6728348843	7.1762987390
H13	-2.8068045449	-2.4150080722	7.3511504048
H14	-4.5950847016	-1.4663469892	5.8965486707
H15	-4.3192249550	0.8034778043	4.9276952121
H16	-2.2562344483	2.1253353516	5.4141978853
H17	2.6333766874	1.0530273555	5.3251807972
H18	3.8749157884	-1.0416672739	4.7566558129
H19	3.1955074747	-3.1947645282	5.7878607363
H20	1.2609397309	-3.2762203469	7.3424522438
C21	-0.3567771627	0.4437133669	11.5327052340
C22	-0.1150693599	1.7760469689	11.1980126290
C23	0.0711799370	2.1415889568	9.8639352034
C24	-0.0209279253	1.1695654610	8.8716937984
C25	-0.2703693441	-0.1705354782	9.1983754516
C26	-0.4273864380	-0.5303602722	10.5351233758

H27	-0.4885825628	0.1593195188	12.5736410597
H28	-0.0556069445	2.5301262955	11.9782538924
H29	0.3004837166	3.1676258262	9.5825344403
H30	-0.6139008445	-1.5703456368	10.7963765695
C31	-0.4067500626	-1.1636933957	8.0498044559
H32	-0.6059141854	-2.1685797684	8.4378690935
N33	-0.1232021482	2.8267402185	6.2054852694
P34	0.5472926066	4.2701559482	6.3066655174
O35	0.6496875064	5.0461005010	7.5651689548
O36	-0.3002805764	5.2096895817	5.2355422171
O37	1.9756917238	4.1797096992	5.4676343767
C38	-0.1227253927	4.9375931015	1.0906359537
C39	-0.1738359953	6.1733886275	1.7370441514
C40	-0.2331567405	6.2366317659	3.1250630167
C41	-0.2466989705	5.0593395392	3.8770605657
C42	-0.2064459413	3.8153355206	3.2421369815
C43	-0.1407199981	3.7682335209	1.8502467139
H44	-0.0679703316	4.8871914351	0.0066975392
H45	-0.1514976478	7.0939288099	1.1595824978
H46	-0.2415680716	7.1847612659	3.6544876645
H47	-0.2149767927	2.9129498397	3.8453019839
H48	-0.1029319678	2.8001394705	1.3573470789
C49	3.9436221383	7.5007435782	3.9231222831
C50	3.8138220456	6.3258614801	3.1812981817
C51	3.1449584691	5.2290336860	3.7146839495
C52	2.6090211640	5.3010779237	5.0023652374
C53	2.7326718387	6.4693410382	5.7575175217
C54	3.3991383425	7.5623034314	5.2054806211
H55	4.4603052749	8.3600452451	3.5045377192
H56	4.2214963458	6.2666013636	2.1755424995

H57	3.0020014127	4.3148908401	3.1456580359
H58	2.2943463677	6.5036262032	6.7500614446
H59	3.4927694462	8.4737630436	5.7905042522
P60	0.2590960206	1.5184773576	7.0914105264
F61	1.7986797919	2.2225325958	7.5729896189

11-He$_8$-ring complex at 1.7 Å

E(BP86/6-31G*) = -2181.474257995

He1	2.0197999498	1.8632999890	11.4446999196
He2	6.2280000760	3.2546000214	9.1307001511
He3	4.8859999848	0.1785001905	10.2418000133
He4	3.3617999032	4.9395000011	10.3335998496
He5	3.1955000232	0.3896000072	11.1134000502
He6	5.0726000363	4.7344000102	9.5021000721
He7	6.1504000036	1.3673998737	9.4371998190
He8	2.0974001058	3.7504999751	11.1382000945
X9	4.1239000000	2.5590000000	10.2877000000
C10	1.0205755206	-0.6841358194	4.8018478619
C11	2.0922937379	-0.5823117671	3.9011493279
C12	3.2792376681	0.0576701273	4.2892578726
C13	3.3901150562	0.6346852511	5.5635139491
C14	2.3081766571	0.5551395382	6.4511398843
C15	2.0113425510	-0.5861730595	8.8506497760
C16	2.8349350911	-1.4495392828	9.5916171818
C17	2.4443410464	-2.7697012917	9.8753544012

C18	1.2256531316	-3.2653001394	9.4048942940
C19	0.4349835692	-2.4500167059	8.5835411973
C20	0.8266574868	-1.1402526323	8.2759930700
C21	1.1315083669	-0.1341610380	6.0866564041
H22	0.1029154261	-1.2120508889	4.5141571688
H23	2.0049118532	-1.0182151666	2.8994965222
H24	4.1230244413	0.1207338854	3.5931613430
H25	4.3070907162	1.1577309812	5.8519727794
H26	3.8014670957	-1.1262177539	9.9528245722
H27	3.1127840236	-3.4045102318	10.4672967872
H28	0.9086179262	-4.2880327625	9.6371308556
H29	-0.4874029181	-2.8428260608	8.1387678559
C30	-2.1413437519	2.5535311083	8.3532134773
C31	-1.1660619848	3.3904480889	8.9184126884
C32	0.1850298106	3.0107766007	8.9030007581
C33	0.5437714775	1.7849158029	8.3257301913
C34	-0.4288597230	0.9431560883	7.7564855900
C35	-1.7760040364	1.3293954015	7.7695463155
H36	-3.1947055865	2.8561131769	8.3644294574
H37	-1.4549049467	4.3467976299	9.3678487800
H38	0.9536786185	3.6634639794	9.3237570576
H39	-2.5373622755	0.6767762132	7.3249014436
C40	0.0830071613	-0.3654139628	7.1838891207
H41	-0.7502331587	-0.9731234431	6.7935250380
P42	2.2744328117	1.1896731083	8.2021559088
N43	3.3659999174	2.3453999317	8.7810000307
P44	3.3991151305	3.4507299152	7.4907123236
O45	3.2171070768	4.9575319697	8.1318348865
O46	2.4657242780	3.2634245530	6.3194010810
O47	5.0001099948	3.4338346182	7.0589787074

C48	1.3381226599	8.3587028019	6.5415709746
C49	2.5669585786	8.4455904253	7.2157593194
C50	3.1893840112	7.2899008518	7.7078436009
C51	2.5724394264	6.0418308323	7.5252367980
C52	1.3405659776	5.9351893356	6.8591507046
C53	0.7362986567	7.1026894068	6.3669707567
H54	0.8542323488	9.2626534281	6.1552769825
H55	3.0510328702	9.4185308124	7.3594987850
H56	4.1491895942	7.3358761342	8.2313105157
H57	0.8865319685	4.9535485011	6.7119517638
H58	-0.2223572013	7.0219724334	5.8409777615
C59	6.7907517388	6.1013753450	4.3489658553
C60	7.4391947514	5.7229813946	5.5357776618
C61	6.8155130223	4.8503991216	6.4392391148
C62	5.5374444791	4.3515776560	6.1425926531
C63	4.8774931392	4.7098206956	4.9550560827
C64	5.5128463530	5.5929761911	4.0683988014
H65	7.2792753113	6.7865490319	3.6473105568
H66	8.4379591869	6.1115091893	5.7665610371
H67	7.3044212831	4.5464737340	7.3691151886
H68	3.8838255571	4.3036427693	4.7459608395
H69	4.9981741365	5.8806073385	3.1442292722

11-He$_8$-ring complex at 2.2 Å

E(BP86/6-31G*) = -2181.507275410

He1	2.0198000000	1.8633000000	11.4447000000
He2	6.2280000201	3.2546000057	9.1307000400

He3	4.8859999932	0.1785000544	10.2417999977
He4	3.3618000000	4.9395000000	10.3336000000
He5	3.1955000000	0.3896000000	11.1134000000
He6	5.0726000000	4.7344000000	9.5021000000
He7	6.1503999996	1.3673999741	9.4371999611
He8	2.0974000000	3.7505000000	11.1382000000
X9	4.1239000000	2.5590000000	10.2877000000
C10	-0.8961456259	-0.2350091010	5.4181810663
C11	-0.3027072034	-0.1941615511	4.1457996959
C12	0.9695987903	0.3691002530	3.9871145215
C13	1.6479172880	0.9228348844	5.0866462208
C14	1.0466561574	0.9068980484	6.3527999186
C15	1.5807755643	-0.1924496255	8.7460979170
C16	2.6326150884	-1.0314574533	9.1269888730
C17	2.3569023943	-2.3330093851	9.5785759328
C18	1.0345257054	-2.7939790070	9.6325359589
C19	-0.0151741206	-1.9787753917	9.1759211011
C20	0.2536516680	-0.6877666488	8.7050573834
C21	-0.2248613744	0.2958823898	6.5266145096
H22	-1.8817236436	-0.6969610849	5.5550735938
H23	-0.8334169925	-0.6141239998	3.2837106327
H24	1.4439013649	0.3911603473	2.9996352155
H25	2.6160994862	1.4056638440	4.9512139858
H26	3.6586026359	-0.6733854874	9.0574022324
H27	3.1815179085	-2.9869684497	9.8831398580
H28	0.8189096364	-3.8052189948	9.9956767544
H29	-1.0426035684	-2.3618982956	9.1521119963
C30	-2.1722152690	3.4057981257	9.4913653480
C31	-1.0037143825	4.1826068099	9.5219547219
C32	0.2173595679	3.6393918392	9.0900076465

C33	0.2464007728	2.3162435588	8.6302019031
C34	-0.9283967573	1.5387138218	8.5692038448
C35	-2.1400504621	2.0850818456	9.0116083964
H36	-3.1211877308	3.8337866592	9.8341972252
H37	-1.0406359631	5.2164377972	9.8824536857
H38	1.1365978784	4.2317818480	9.1075140487
H39	-3.0588007416	1.4871393963	8.9713082043
C40	-0.7842055044	0.1530681626	7.9546177891
H41	-1.7561924987	-0.3672870714	7.9318147794
P42	1.7457282589	1.4800500976	7.9987573518
N43	3.1444999871	2.2828999659	8.3406000012
P44	3.4870463572	3.3865973120	7.1436303143
O45	3.3609964699	4.8560816117	7.8981463948
O46	2.7280856188	3.3868880952	5.8414984090
O47	5.1111485464	3.1543192295	6.9644431309
C48	2.4943533219	8.5907283998	6.1936545069
C49	3.5965619251	8.4208257617	7.0464278226
C50	3.8924957632	7.1584044159	7.5794174034
C51	3.0737496790	6.0654116979	7.2545728291
C52	1.9615124959	6.2183478429	6.4101240735
C53	1.6849052017	7.4876978992	5.8797032426
H54	2.2669273739	9.5781183841	5.7765427589
H55	4.2362962725	9.2743410402	7.2985620209
H56	4.7487675729	7.0050472996	8.2423160170
H57	1.3487171060	5.3492051302	6.1615592130
H58	0.8215874032	7.6115119339	5.2154930875
C59	7.7631419329	5.1435701795	4.3859464597
C60	8.2203412841	4.3897187447	5.4787875447
C61	7.3102251533	3.7454225767	6.3267965636
C62	5.9318769975	3.8546966007	6.0749230142

C63	5.4573885415	4.5923356335	4.9766773467
C64	6.3847256935	5.2375066564	4.1437270563
H65	8.4765512205	5.6495923354	3.7261558713
H66	9.2945392252	4.3020645897	5.6788410984
H67	7.6487902264	3.1540257551	7.1819256440
H68	4.3846435529	4.6460328775	4.7741283279
H69	6.0151630366	5.8174203652	3.2900990538

12

E(M06-2X/6-311+G**) = -2261.734802708

H(M06-2X/6-31+G*) = -2261.73480270839

E(BP86/6-31G*) = -2262.024470782

C1	-0.9135887972	-0.9698017055	5.4066405007
C2	-0.4245152573	-0.8413590506	4.1037224050
C3	0.6409575759	0.0106375316	3.8278655921
C4	1.2405748984	0.7470088543	4.8531564695
C5	0.7544385633	0.6066005963	6.1483438637
C6	1.5340700844	-0.0172057195	8.7208414113
C7	2.6612493819	-0.3473817348	9.4600888957
C8	2.6257781678	-1.4964647213	10.2531374972
C9	1.4771072815	-2.2834670094	10.2919683590
C10	0.3473615843	-1.9405761865	9.5428537203
C11	0.3718481085	-0.7998975507	8.7502872277
C12	-0.3275031219	-0.2446382718	6.4365492149
H13	-1.7497816083	-1.6322498736	5.6154324071
H14	-0.8856294900	-1.4087910608	3.3006783515
H15	1.0058573812	0.1122652229	2.8107941613

H16	2.0507418181	1.4412636546	4.6492379674
H17	3.5417394934	0.2874858472	9.4121967505
H18	3.4945947005	-1.7751876010	10.8412560612
H19	1.4563257718	-3.1746921608	10.9121074129
H20	-0.5446209291	-2.5605817493	9.5808325843
C21	-2.7051471533	2.7375617803	9.2286802639
C22	-1.7173777477	3.7147165498	9.1473842596
C23	-0.4445722904	3.3944575518	8.6671735397
C24	-0.1937389608	2.0840687676	8.2770831249
C25	-1.1843554389	1.0892604211	8.3496684569
C26	-2.4441370895	1.4230856050	8.8297376879
H27	-3.6910493425	2.9964543106	9.6034355635
H28	-1.9348554463	4.7330285846	9.4544581670
H29	0.3350064968	4.1471542102	8.5805406843
H30	-3.2214366963	0.6657286119	8.8940146729
C31	-0.7957483632	-0.3173778269	7.8906776594
H32	-1.6468813386	-0.9975191218	7.9823521633
P33	1.3788389472	1.4271207958	7.6485867444
N34	2.7314178596	2.2683204949	7.6812793078
S35	2.9723560382	3.6502624873	6.8629725973
O36	2.2350657934	4.7623876285	7.4696962725
O37	2.7313624951	3.4662750635	5.4264063687
C38	7.4568281693	4.5735821903	7.1053273807
C39	6.5731237434	5.1415808075	8.0207757410
C40	5.2175346602	4.8093117726	8.0673978203
C41	4.7422802778	3.8958072987	7.1014139081
C42	5.6245199153	3.2034900895	6.2473068720
C43	6.9695112422	3.5816654304	6.2607510109
H44	6.9497128830	5.8712446667	8.7332599540
C45	4.3796206738	5.4321308279	9.1823895922

C46	5.2316749058	2.0392149279	5.3421447119
H47	7.6619280197	3.0824569720	5.5864976556
C48	8.9119900209	4.9961082880	7.0570725375
H49	9.3973958439	4.4031691653	6.2712194532
C50	9.0450402554	6.4770195730	6.6833201878
H51	8.5941300814	7.1143430320	7.4520934250
H52	10.0999624965	6.7575179382	6.5912932551
H53	8.5449957860	6.6920966300	5.7342193568
C54	5.2273288429	2.4564853115	3.8679971209
C55	6.1474683659	0.8285682757	5.5727957400
H56	4.2249426566	1.7162544862	5.6036423716
H57	3.4567195985	4.8629597574	9.2836061071
C58	5.0977892986	5.3610660575	10.5377560557
C59	4.0068262773	6.8795822986	8.8434395017
H60	5.7640851986	-0.0314325918	5.0130672402
H61	7.1722833683	1.0104093978	5.2317521296
H62	6.1839932620	0.5576455089	6.6332445200
H63	4.9206217927	1.6140837112	3.2366671520
H64	4.5333640433	3.2847937389	3.7055631273
H65	6.2296023423	2.7672438270	3.5487564229
H66	10.6906649773	4.9571556660	8.3080452532
C67	9.6277546715	4.7027496309	8.3806934211
H68	9.1971072398	5.2949088388	9.1955889150
H69	9.5420836950	3.6461432302	8.6515758115
H70	3.3958772191	7.3121794368	9.6441456350
H71	4.9095336463	7.4939854648	8.7366451264
H72	3.4374057742	6.9251906940	7.9123264068
H73	4.4021180765	5.6570852585	11.3304936109
H74	5.4492349083	4.3466076595	10.7529518213

12-H$^+$

E(M06-2X/6-311+G**) = -2262.114074290

H(M06-2X/6-31+G*) = -2261.021577

C1	-0.6119907249	-1.0579955406	5.3297367438
C2	-0.0200438781	-0.9144581896	4.0730350202
C3	1.0647024647	-0.0612155791	3.8952384900
C4	1.5796357011	0.6617509145	4.9715777765
C5	0.9931586443	0.5018034022	6.2227089816
C6	1.5322467893	-0.1945314252	8.8709254872
C7	2.5982277256	-0.5684703480	9.6810649154
C8	2.4822638380	-1.7370094451	10.4348673052
C9	1.3222958843	-2.5044562493	10.3598763117
C10	0.2633906711	-2.1270707931	9.5295402475
C11	0.3620157128	-0.9647392374	8.7765836985
C12	-0.1132348834	-0.3524111675	6.4169530470
H13	-1.4643145421	-1.7188301721	5.4606054386
H14	-0.4164980397	-1.4687399829	3.2283594681
H15	1.5104043693	0.0566566943	2.9129971528
H16	2.3974790236	1.3564171716	4.8249523923
H17	3.5125823288	0.0174540323	9.7234628598
H18	3.3003841142	-2.0481322938	11.0758191361
H19	1.2407479149	-3.4120378462	10.9494467624
H20	-0.6319304535	-2.7395871916	9.4713971956
C21	-2.7734599170	2.5510433023	9.0393389244
C22	-1.7904073840	3.5361422685	9.0782417969
C23	-0.4757780362	3.2371639285	8.7152875961
C24	-0.1854002791	1.9354674216	8.3196757312

C25	-1.1678669904	0.9298424769	8.2728936897
C26	-2.4687564938	1.2471366446	8.6372109921
H27	-3.7920812347	2.7968221878	9.3225248991
H28	-2.0441562829	4.5447881522	9.3870336119
H29	0.2932204082	4.0036884405	8.7269285616
H30	-3.2443681322	0.4868672930	8.6089518136
C31	-0.7197059797	-0.4610564347	7.8200969815
H32	-1.5676811893	-1.1490101041	7.8081200037
P33	1.3976893973	1.2519895540	7.8114217230
S34	3.0106281427	3.6960965053	7.1696749042
O35	2.3119808322	4.7062668395	7.9376561976
O36	2.5412264653	3.3965086832	5.8307548582
C37	7.4475341969	4.6489014527	6.9412831310
C38	6.6557275300	5.2301155742	7.9314840660
C39	5.3197128256	4.8915034802	8.1370757833
C40	4.7715769372	3.9278867474	7.2485199135
C41	5.5671703517	3.2209953618	6.3142347145
C42	6.8946125443	3.6230381746	6.1786636908
H43	7.0968493728	5.9833057700	8.5769536656
C44	4.6039606969	5.5730729308	9.3039863269
C45	5.1003404125	2.0321962239	5.4807937725
H46	7.5228259203	3.1172329371	5.4503326552
C47	8.8791854918	5.0950609468	6.7337120121
H48	9.2898256047	4.5023007981	5.9070702802
C49	8.9393378411	6.5753985794	6.3358067053
H50	8.5707771651	7.2153105649	7.1453017099
H51	9.9724120198	6.8679441131	6.1247303775
H52	8.3365547002	6.7750940567	5.4449171940
C53	4.8954873239	2.4248528586	4.0129509722
C54	6.0741176831	0.8511980623	5.6030910024

H55	4.1497903652	1.6788303703	5.8800451730
H56	3.7197301806	4.9943181760	9.5700052709
C57	5.4836168131	5.6301280798	10.5618657147
C58	4.1436216340	6.9822155150	8.9071951937
H59	5.6363105439	-0.0297112674	5.1226395755
H60	7.0296793282	1.0491162961	5.1087627350
H61	6.2771852816	0.6054007733	6.6503555198
H62	4.5636519736	1.5562240724	3.4325213178
H63	4.1520056492	3.2195409818	3.9118587783
H64	5.8361984092	2.7743470379	3.5737848829
H65	10.7726448374	5.0972704077	7.7939137675
C66	9.7293790965	4.8260248931	7.9820735445
H67	9.3788919782	5.4218784552	8.8322729498
H68	9.6950561990	3.7707855265	8.2696486934
H69	3.6176331779	7.4548009085	9.7428531884
H70	5.0081269944	7.6069370788	8.6552151245
H71	3.4702063296	6.9583717870	8.0474275530
H72	4.8701413087	5.9497365954	11.4098380461
H73	5.9167274811	4.6537821140	10.8019656399
H74	6.3005243867	6.3520639374	10.4704062792
N75	2.7815653372	2.1769071940	7.9918407587
H76	3.1210414533	2.2092860149	8.9565010129

12-Me$^+$

E(M06-2X/6-311+G**) = -2301.412304985

H(M06-2X/6-31+G*) = xxxx

C1	-0.6584272642	-0.7517035854	5.1600265321
C2	-0.2257027490	-0.3846296962	3.8848323701
C3	0.7723678098	0.5708003754	3.7339951334
C4	1.3470431204	1.1802052330	4.8504139454
C5	0.9139104447	0.8101807204	6.1198155012
C6	1.8039446604	-0.2628631410	8.5127932489
C7	3.0185154631	-0.6793520917	9.0476505393
C8	3.1213295381	-1.9841064765	9.5306518338
C9	2.0246908912	-2.8416605463	9.4664400114
C10	0.8178869085	-2.4210838563	8.9018925908
C11	0.7027579948	-1.1256203131	8.4145800874
C12	-0.0959703587	-0.1678396656	6.2876400958
H13	-1.4378656779	-1.4993194592	5.2782923939
H14	-0.6736820415	-0.8475091655	3.0113395973
H15	1.1069712031	0.8612782035	2.7434166838
H16	2.0984220016	1.9457709247	4.7209217630
H17	3.8729472695	-0.0087579393	9.0818359998
H18	4.0584380028	-2.3301740087	9.9542015836
H19	2.1115522465	-3.8539712435	9.8483092034
H20	-0.0232996612	-3.1049406941	8.8354147046
C21	-2.6971542873	1.9803172936	9.5834695307
C22	-1.8093641723	3.0517654513	9.6644474982
C23	-0.5230630653	2.9394980848	9.1344419422
C24	-0.1648026720	1.7353280322	8.5367560894
C25	-1.0524930910	0.6546927547	8.4325817928
C26	-2.3285187791	0.7818755713	8.9644574894
H27	-3.6950055203	2.0793783764	9.9992245169
H28	-2.1194340573	3.9793128286	10.1341902020
H29	0.1705264384	3.7769809034	9.1672560172
H30	-3.0361805928	-0.0396176044	8.8953707690

C31	-0.5313262072	-0.5788364706	7.6993190646
H32	-1.3075449419	-1.3446266897	7.6380839006
P33	1.4165407627	1.3418612804	7.7879340869
S34	2.9002931190	3.8954724528	7.3116291277
O35	2.2591111770	4.9364715460	8.0892721642
O36	2.4022779827	3.6154255972	5.9778088338
C37	7.4441480463	4.3213915220	7.0566680035
C38	6.7081238035	5.1704869157	7.8817066862
C39	5.3298011041	5.0584286493	8.0625622488
C40	4.6790132645	4.0265069309	7.3322201683
C41	5.3947466273	3.0959407776	6.5393425308
C42	6.7710509668	3.2836957656	6.4197317178
H43	7.2305358642	5.9610259129	8.4100139539
C44	4.6663605717	6.0730377878	8.9945369976
C45	4.8030038526	1.8991375673	5.7980918516
H46	7.3400830573	2.5961955525	5.7998681069
C47	8.9340219218	4.5180399853	6.8733420799
H48	9.2891610653	3.7221632585	6.2069181378
C49	9.2270395789	5.8667210008	6.2035437158
H50	8.9144599600	6.6988356209	6.8443262634
H51	10.3004354512	5.9725396890	6.0192969921
H52	8.7029575538	5.9604701462	5.2477598477
C53	4.7679951150	2.1637667777	4.2879164258
C54	5.5609075572	0.6036411826	6.1177090820
H55	3.7787560389	1.7355618884	6.1251467334
H56	3.7781367222	5.6212730979	9.4337353656
C57	5.5682122591	6.4911682791	10.1637910749
C58	4.2267789279	7.3112731302	8.1989902977
H59	5.0115507842	-0.2506545602	5.7081296001
H60	6.5624577018	0.5895469679	5.6781121696

H61	5.6665669812	0.4590754520	7.1981252292
H62	4.3388302354	1.3028763960	3.7629036162
H63	4.1710999167	3.0515849259	4.0577440235
H64	5.7787548905	2.3224812779	3.8975569607
H65	10.7600649818	4.4722073264	8.0442969700
C66	9.6809469792	4.3921033993	8.2069124007
H67	9.3894383581	5.1901662517	8.8987545466
H68	9.4767945604	3.4319452699	8.6906478268
H69	3.7343328054	8.0281094157	8.8635714736
H70	5.0991498334	7.8032440188	7.7539474651
H71	3.5272884642	7.0553290093	7.3995758191
H72	4.9651737955	7.0376879702	10.8950035872
H73	6.0148761975	5.6282081617	10.6688617660
H74	6.3742971194	7.1634306102	9.8536947925
N75	2.6366654751	2.4224636728	8.1847903591
C76	2.9463033071	2.5594415838	9.6338153759
H77	2.4500080411	3.4415494026	10.0450048643
H78	2.6062340387	1.6763546683	10.1755763464
H79	4.0305109469	2.6519772020	9.7457329207

12-F^-

E(M06-2X/6-311+G**) = -2361.6713539541

H(M06-2X/6-31+G*) = -2360.562273

C1	0.1882778143	-1.6113753293	6.3799170547
C2	0.2708076508	-1.5757451032	4.9867051752
C3	0.5304191237	-0.3736699921	4.3288106082
C4	0.7206430153	0.7990856203	5.0610102165

C5	0.6185714768	0.7616543504	6.4482197286
C6	1.8469762716	1.4912260468	8.9004504079
C7	2.9575157098	2.0907129564	9.4918534464
C8	3.6459131636	1.4248686407	10.5067071136
C9	3.2512951471	0.1459451589	10.8971944216
C10	2.1592914927	-0.4675521660	10.2824466558
C11	1.4468482550	0.2048552901	9.2917960683
C12	0.3520761796	-0.4404996566	7.1169834571
H13	-0.0135989932	-2.5495864679	6.8931847723
H14	0.1330514097	-2.4898836603	4.4147704429
H15	0.5973995586	-0.3514933552	3.2443350713
H16	0.9586522898	1.7416861627	4.5725563489
H17	3.2905029015	3.0684318191	9.1495006824
H18	4.5006885001	1.9001761523	10.9802680097
H19	3.7967366999	-0.3784204843	11.6776503881
H20	1.8541307072	-1.4691025546	10.5794806695
C21	-3.0716762433	1.1531768182	9.8864359686
C22	-2.9091047657	2.4576492919	9.4270219611
C23	-1.7600371774	2.8219990942	8.7165354489
C24	-0.7596476646	1.8855077609	8.4607482717
C25	-0.9369107074	0.5771229477	8.9339745206
C26	-2.0769577756	0.2045486333	9.6372830796
H27	-3.9667596326	0.8715776770	10.4357295479
H28	-3.6817204124	3.1987450945	9.6180779607
H29	-1.6281925174	3.8336870071	8.3441362206
H30	-2.1888175909	-0.8188788529	9.9910234987
C31	0.2050414136	-0.3818106218	8.6321335239
H32	-0.0014098151	-1.3802102725	9.0328113264
N33	0.4189759811	3.7734661780	7.2139837649
S34	1.2260479369	4.8903269023	6.3909698135

O35	0.4505646199	6.1386091111	6.4589737451
O36	1.6064609009	4.4836091418	5.0325073145
C37	4.8692065645	5.7295966318	9.1391538704
C38	3.5577569766	5.9277159903	9.5576428277
C39	2.4625348322	5.6833058803	8.7240598926
C40	2.7084303612	5.2174637497	7.4127103493
C41	4.0250128399	4.9797558876	6.9633605101
C42	5.0747157803	5.2565093377	7.8469830919
H43	3.3676362563	6.2773981169	10.5705226697
C44	1.0829751114	5.9399059790	9.3336072839
C45	4.3772171447	4.4762051120	5.5679606392
H46	6.0970558818	5.0856318323	7.5198837991
C47	6.0434229259	5.9603026936	10.0704429432
H48	6.9533826554	5.9486248717	9.4548730935
C49	5.9768415751	7.3154451309	10.7811679544
H50	5.1224197581	7.3621280803	11.4655613885
H51	6.8844690615	7.4847196605	11.3724157433
H52	5.8735380684	8.1329555929	10.0607260503
C53	4.4358460421	5.6549759100	4.5874717679
C54	5.6804920057	3.6734457089	5.5201270563
H55	3.5787357693	3.8101541745	5.2494337012
H56	0.3129502622	5.6896776556	8.6109556427
C57	0.8411657826	5.0531083443	10.5600025775
C58	0.9158285246	7.4277562953	9.6632546994
H59	5.7668202805	3.1952910077	4.5380515725
H60	6.5724010652	4.2990742356	5.6529628485
H61	5.6884829276	2.8855781534	6.2810447319
H62	4.6532464567	5.2954338349	3.5742018518
H63	3.4797903086	6.1841489172	4.5597065747
H64	5.2255387721	6.3610973819	4.8787489880

H65	7.0148723937	4.9554171134	11.7482751506
C66	6.1507756654	4.8165719915	11.0871470786
H67	5.2474186183	4.7713330195	11.7075614205
H68	6.2545181306	3.8535324623	10.5764937686
H69	-0.0908353117	7.6136639493	10.0560435524
H70	1.6390478977	7.7660232063	10.4164016602
H71	1.0471021340	8.0304306505	8.7591812321
H72	-0.1637268789	5.2370212816	10.9586788228
H73	0.9016905202	3.9933253288	10.2898193275
H74	1.5631453968	5.2436662262	11.3638896124
P75	0.8783473335	2.2329595234	7.5114020570
F76	2.4342562223	2.4390009190	6.7205933016

12-He$_8$-ring complex at 1.7 Å

E(BP86/6-31G*) = -2285.098791888

He1	2.0198000211	1.8632999921	11.4447000052
He2	6.2279999486	3.2545999825	9.1307000627
He3	4.8860000000	0.1785000000	10.2418000000
He4	3.3618000498	4.9395000140	10.3336000990
He5	3.1955000000	0.3896000000	11.1134000000
He6	5.0725999818	4.7344000133	9.5020998903
He7	6.1504000000	1.3674000000	9.4372000000
He8	2.0973999725	3.7504999944	11.1381999586
X9	4.1239000000	2.5590000000	10.2877000000
C10	-1.3675913151	3.8771253698	5.8474513331
C11	-1.3629543642	3.0007422235	4.7507937967
C12	-0.3453692907	2.0493917953	4.6402695050

C13	0.6792129882	1.9801552459	5.6026056878
C14	0.6913752816	2.8587943292	6.6916751422
C15	0.4695054117	2.7687330948	9.3463982051
C16	0.2146347288	1.6014376545	10.0781005876
C17	-0.9681866439	1.4866194882	10.8267793257
C18	-1.9056262365	2.5294839849	10.8316035901
C19	-1.7026048766	3.6507663579	10.0106228746
C20	-0.5382839146	3.7551953879	9.2365318980
C21	-0.3646163161	3.8098326672	6.8221318952
H22	-2.1666135461	4.6208271812	5.9574649500
H23	-2.1553412054	3.0625210046	3.9962270239
H24	-0.3286395018	1.3502249373	3.7965430407
H25	1.4799063290	1.2540669052	5.4865884868
H26	0.9385290612	0.7846253172	10.0740077580
H27	-1.1531054043	0.5757518773	11.4071340816
H28	-2.8184152325	2.4492345195	11.4323615164
H29	-2.4747610264	4.4258866986	9.9316159512
C30	2.0877968023	7.6041165724	7.6739095144
C31	3.2758896887	6.8663547940	7.5532590365
C32	3.2674384719	5.4733640269	7.7273135186
C33	2.0559965921	4.8337081479	8.0213922138
C34	0.8471778500	5.5557573226	8.0550848418
C35	0.8674289617	6.9492048697	7.9078196003
H36	2.1044308796	8.6933191022	7.5521931357
H37	4.2171669214	7.3765598563	7.3202566923
H38	4.1824610931	4.8839192023	7.6220705441
H39	-0.0706015974	7.5169589070	7.9426066762
C40	-0.4235491929	4.7238792942	8.0636423225
H41	-1.3146518538	5.3724143472	8.0136097195
P42	1.8998411451	3.0153184376	8.1958340694

N43	3.3660000262	2.3454000037	8.7809999842
S44	4.2280987750	1.8025464029	7.3637256129
O45	5.3394023053	2.7536195745	7.1010196865
O46	3.2869696783	1.6206861206	6.2109323399
C47	5.8152200585	-2.6175357512	7.6805543873
C48	6.6967660335	-1.5516157038	7.4591335740
C49	6.2912231137	-0.2027175610	7.4118477181
C50	4.8985895587	0.0756264917	7.5930072621
C51	3.9661698686	-0.9872095329	7.7757434117
C52	4.4614851363	-2.3034470370	7.8308696836
H53	7.7602274437	-1.7694619580	7.3136402243
C54	7.4018222779	0.8184082766	7.1066512365
C55	2.4381327428	-0.8562515604	7.8329749064
H56	3.7484397336	-3.1234963222	7.9761518034
C57	6.2945291268	-4.0657021809	7.7414509328
H58	5.3996760413	-4.6951292156	7.9205905975
C59	6.9222160176	-4.5181855141	6.4041394911
H60	7.8329833239	-3.9362600452	6.1723066790
H61	7.2088821206	-5.5849043015	6.4498191302
H62	6.2165633116	-4.3861553371	5.5653742395
C63	1.8277683616	-1.3596684790	6.5036060625
C64	1.8089175243	-1.6114285189	9.0249149682
H65	2.1745667861	0.2050191744	7.9441626135
H66	7.0726985123	1.8067066688	7.4440594748
C67	8.7357370884	0.5102297388	7.8229614628
C68	7.6113004221	0.9173097228	5.5771803645
H69	0.7224013859	-1.4109328121	9.0610841051
H70	1.9284508488	-2.7059746277	8.9360997486
H71	2.2531648539	-1.3039152738	9.9856360429
H72	0.7378408545	-1.1762916837	6.4825418673

H73	2.2881922318	-0.8491766132	5.6420213314
H74	1.9924985276	-2.4464214462	6.3829397175
H75	7.5593318332	-5.3601584625	8.9817133146
C76	7.2692892522	-4.2952610171	8.9181160943
H77	8.1939241267	-3.7026398817	8.7926093546
H78	6.8117772258	-4.0044381135	9.8799591952
H79	8.4011981648	1.6559888856	5.3472300814
H80	7.9191546916	-0.0563643375	5.1513666124
H81	6.6861214594	1.2406360962	5.0714419234
H82	9.4145188593	1.3750554397	7.7109385013
H83	8.5900147433	0.3314951761	8.9031634484
H84	9.2640374731	-0.3647379255	7.4010070347

12-He$_8$-ring complex at 2.2 Å

E(BP86/6-31G*) = -2285.134475939

He1	2.0197999236	1.8632999806	11.4446998610
He2	6.2280001122	3.2546000316	9.1307002230
He3	4.8860000000	0.1785000000	10.2418000000
He4	3.3617997895	4.9394997485	10.3335993678
He5	3.1955000441	0.3896000137	11.1134000956
He6	5.0725999564	4.7343997820	9.5020999641
He7	6.1504000000	1.3674000000	9.4372000000
He8	2.0974001519	3.7505000287	11.1382006820
X9	4.1239000000	2.5590000000	10.2877000000
C10	4.2825276112	0.2994127521	3.1634562817
C11	3.1285180939	0.6872707760	2.4632492653
C12	2.1048188745	1.3624613841	3.1366506528

C13	2.2160681666	1.6444439714	4.5106819532
C14	3.3635569844	1.2577491036	5.2147574602
C15	5.4258258546	2.3207871514	6.6066195472
C16	5.7189639599	3.6618362654	6.8719363434
C17	6.9238138741	4.2073734040	6.4005003780
C18	7.8171110291	3.4093431226	5.6679510194
C19	7.4865919126	2.0795092497	5.3500683551
C20	6.2737785387	1.5357201207	5.7962329424
C21	4.4155244745	0.5846118533	4.5279096481
H22	5.0936081588	-0.2261358078	2.6448255421
H23	3.0365647936	0.4603766976	1.3949801729
H24	1.1999605744	1.6705380547	2.6012576703
H25	1.4011267466	2.1363122919	5.0409312139
H26	4.9956287713	4.2490854737	7.4447642405
H27	7.1663594533	5.2564021813	6.6057146187
H28	8.7628240156	3.8326412234	5.3111439223
H29	8.1579510808	1.4767877865	4.7256476100
C30	5.1545812461	-2.8728855682	7.5477893404
C31	4.1551141707	-2.3828435210	8.4022327755
C32	3.7318795205	-1.0467898531	8.3046539310
C33	4.3224903579	-0.2214393116	7.3382931674
C34	5.2869616672	-0.7199381196	6.4365888403
C35	5.7169223151	-2.0478710367	6.5572953959
H36	5.4870211892	-3.9133480928	7.6365864735
H37	3.7004973666	-3.0426831198	9.1498514665
H38	2.9513434043	-0.6461437226	8.9607368495
H39	6.4706235434	-2.4452854151	5.8657441664
C40	5.6976556654	0.2100026425	5.2978583343
H41	6.4100467478	-0.2928543665	4.6231776263
P42	3.8390784136	1.5167913069	7.0340487512

N43	3.1432000222	2.2826004150	8.3378998064
S44	1.4494781986	2.1055271033	8.3583028773
O45	1.1144036977	1.1023651975	9.4011837662
O46	0.9137063611	1.8084263924	6.9895993153
C47	-0.4906524466	6.2947931913	9.2654926536
C48	-0.8373174576	5.1592619342	10.0115104654
C49	-0.2753793510	3.8859902346	9.7965335216
C50	0.7201961231	3.7640561110	8.7731553018
C51	1.0450100454	4.8821620342	7.9513929230
C52	0.4378509739	6.1198070131	8.2366698531
H53	-1.5898645001	5.2584187550	10.7996955699
C54	-0.8528184371	2.7299724484	10.6290553239
C55	1.9316327467	4.8621563010	6.7016491026
H56	0.6911408035	6.9820044900	7.6085165355
C57	-1.1123799527	7.6624143378	9.5366529124
H58	-0.6804131802	8.3657823968	8.7968489916
C59	-2.6429098551	7.6486480869	9.3281861640
H60	-3.1380566981	6.9734208540	10.0480405139
H61	-3.0646824886	8.6595260110	9.4738960774
H62	-2.9066607814	7.3070361667	8.3118219244
C63	1.0446003745	4.9484411392	5.4365215854
C64	2.9885852179	5.9906572288	6.6985969932
H65	2.4748408609	3.9086131620	6.6668959427
H66	-0.0659557610	1.9820595802	10.7744062998
C67	-1.3559241104	3.1451848598	12.0272557867
C68	-1.9853650193	2.0398109124	9.8308291990
H69	3.6905872275	5.8496033411	5.8568304223
H70	2.5304103842	6.9899617607	6.5743095671
H71	3.5697163903	6.0050692751	7.6368414908
H72	1.6615142329	4.8516392089	4.5262015661

H73	0.2851084561	4.1480402504	5.4330668117
H74	0.5150343675	5.9176756366	5.3874405025
H75	-1.1570978455	9.2016350892	11.0997909295
C76	-0.7497221198	8.1868435959	10.9450144610
H77	-1.1654372982	7.5354823739	11.7341332231
H78	0.3433180220	8.2289531209	11.0868522234
H79	-2.3917362749	1.1878333199	10.4061166143
H80	-2.8140017950	2.7458870862	9.6306105442
H81	-1.6184523360	1.6534695274	8.8655241628
H82	-1.5755180508	2.2362315751	12.6148331291
H83	-0.6003579185	3.7306326787	12.5808872751
H84	-2.2910863642	3.7346681079	11.9938819403

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E(M06-2X/6-311+G**) = -1359.425808708

H(M06-2X/6-31+G*) = -1358.793312

E(BP86/6-31G*) = -1382.719802199

C1	-2.4978313466	1.2676319689	6.9534286188
C2	-2.8021593964	2.5617242134	6.5204695566
C3	-1.7957007386	3.5081165814	6.3439896418
C4	-0.4642043296	3.1693259235	6.5969856391
C5	-0.1672260550	1.8789076275	7.0182984750
C6	1.4207084779	-0.2785166441	6.4363672680
C7	2.3963910299	-0.7170482562	5.5495491648
C8	2.2052712810	-1.9275494001	4.8788397543
C9	1.0544810130	-2.6779728766	5.1077188188
C10	0.0807454020	-2.2357925786	6.0083252351

C11	0.2607731322	-1.0312428976	6.6770611881
C12	-1.1758790421	0.9206329493	7.2039279872
H13	-3.2905323927	0.5370036338	7.0947866337
H14	-3.8356508614	2.8305731391	6.3229211824
H15	-2.0449621960	4.5108348410	6.0107512323
H16	0.3330592462	3.8977519177	6.4689777131
H17	3.2916266129	-0.1216934436	5.3862240819
H18	2.9560395921	-2.2832349430	4.1799132526
H19	0.9110823777	-3.6186187492	4.5842194198
H20	-0.8115793342	-2.8311258341	6.1859458046
C21	0.3272755658	-0.6810491475	11.3828516891
C22	1.4489810191	0.1451561282	11.3806594466
C23	1.8572083127	0.7667083794	10.1982312446
C24	1.1259230213	0.5428038335	9.0400472834
C25	-0.0055020655	-0.2868212769	9.0285291125
C26	-0.4025677762	-0.8998468492	10.2105865299
H27	0.0138022892	-1.1623092079	12.3046322355
H28	2.0063842536	0.3060445624	12.2982433182
H29	2.7272772764	1.4164247359	10.1629694291
H30	-1.2762160357	-1.5463267010	10.2227006501
C31	-0.7297144557	-0.4580120393	7.6906439944
H32	-1.5908891307	-1.1222166596	7.8049618392
P33	1.5012663268	1.2559915503	7.4240243798
N34	2.7679544740	2.1824966945	7.4461292105
C35	4.5102119503	4.3429366527	4.2654276855
C36	5.0340757007	4.3827671806	5.5593380386
C37	4.4416360249	3.6623636763	6.5883345513
C38	3.2991675421	2.8731135271	6.3595310423
C39	2.7798617266	2.8409379685	5.0500167796
C40	3.3797487001	3.5662159389	4.0225682293

H41	4.9754559422	4.9069897636	3.4631269478
H42	5.9155196915	4.9830187609	5.7691870255
H43	4.8457443383	3.6905865606	7.5959991479
H44	1.8961414754	2.2414974452	4.8317866619
H45	2.9551076513	3.5202450951	3.0231372016

13-H$^+$

E(M06-2X/6-311+G**) = -1359.826619839

H(M06-2X/6-31+G*) = -1359.17756

C1	-2.4207276919	1.3544040934	6.9006374961
C2	-2.6929435673	2.6696194862	6.5126556837
C3	-1.6746378681	3.6155447959	6.4123639807
C4	-0.3558989070	3.2580218770	6.6949093485
C5	-0.0976352138	1.9444596815	7.0702301041
C6	1.5157589763	-0.2483239076	6.4773994076
C7	2.5360609658	-0.6727305774	5.6337849787
C8	2.3585129356	-1.8661372345	4.9330898906
C9	1.1855751329	-2.6019316028	5.0900789233
C10	0.1715036747	-2.1688708210	5.9495436300
C11	0.3305992169	-0.9826024200	6.6535009302
C12	-1.1138289293	0.9804883130	7.1841624802
H13	-3.2266038156	0.6305505945	6.9830418068
H14	-3.7154080379	2.9579567749	6.2903291780
H15	-1.9052028582	4.6330809373	6.1150159560
H16	0.4477871722	3.9860857305	6.6215794703

H17	3.4464142725	-0.0896597505	5.5211501352
H18	3.1373879476	-2.2202413922	4.2660565820
H19	1.0571311888	-3.5288844133	4.5402735211
H20	-0.7333889930	-2.7581060065	6.0686163116
C21	0.1862725858	-0.7819767280	11.3720013661
C22	1.3164441450	0.0264667960	11.4599296831
C23	1.7940086527	0.6852999197	10.3266491519
C24	1.1188719545	0.5136431259	9.1239385005
C25	-0.0253578147	-0.3000363154	9.0189790063
C26	-0.4855229803	-0.9473733356	10.1578617904
H27	-0.1794376675	-1.2914175602	12.2577457451
H28	1.8285249545	0.1464374646	12.4086300075
H29	2.6764489293	1.3148433201	10.4018574880
H30	-1.3660447016	-1.5807848062	10.1033242220
C31	-0.6949475607	-0.4200379878	7.6429708505
H32	-1.5650246462	-1.0770291194	7.7052107833
P33	1.4812602216	1.2164075305	7.5137765259
C34	4.4021986349	4.2808861526	4.1984538867
C35	4.9883669317	4.3778576064	5.4589803034
C36	4.4532140269	3.6863778874	6.5407665375
C37	3.3222665552	2.8910386408	6.3590071155
C38	2.7261311227	2.7859492046	5.1021067082
C39	3.2731099375	3.4847871262	4.0270424390
H40	4.8226384831	4.8216389318	3.3575300395
H41	5.8686097956	4.9949826479	5.6070684900
H42	4.9146068869	3.7664557136	7.5220481387
H43	1.8434702401	2.1704961089	4.9416586415
H44	2.8069712373	3.4006366916	3.0506686822
N45	2.8002211818	2.1951430455	7.4929709116
H46	3.3047209941	2.3236982714	8.3640442218

13-Me$^+$

E(M06-2X/6-311+G**) = -1399.122488853

H(M06-2X/6-31+G*) = -1398.435134

C1	-2.5773619668	1.2310718542	7.1131046723
C2	-2.9828335662	2.5408445810	6.8392452756
C3	-2.0580837945	3.5811521574	6.7774442836
C4	-0.7028436744	3.3243711147	6.9893628614
C5	-0.3099190245	2.0186413021	7.2610536789
C6	1.4882713263	0.0767883760	6.3757355922
C7	2.4726855216	-0.1954763989	5.4285057803
C8	2.3358762915	-1.3318887545	4.6302493484
C9	1.2362582293	-2.1707994669	4.7818038985
C10	0.2569950325	-1.8949507497	5.7385471759
C11	0.3732039116	-0.7713081947	6.5461604753
C12	-1.2320170714	0.9628362761	7.3282174875
H13	-3.3094282777	0.4294692712	7.1555896600
H14	-4.0347423286	2.7490262284	6.6717067625
H15	-2.3902759097	4.5916792687	6.5642314002
H16	0.0261030587	4.1299949604	6.9431453619
H17	3.3324092177	0.4541371504	5.3048651545
H18	3.0943206263	-1.5566883232	3.8878442339
H19	1.1374435269	-3.0505127448	4.1538681498
H20	-0.5952516116	-2.5585040239	5.8548557333
C21	0.4890458632	-1.0894572866	11.2410899465
C22	1.5603386938	-0.2047933304	11.3421109636
C23	1.8969658246	0.6112927040	10.2614055137

C24	1.1368667752	0.5218775735	9.1006535939
C25	0.0637115815	-0.3767102932	8.9798033826
C26	-0.2569878429	-1.1843411089	10.0628051044
H27	0.2332149924	-1.7207231877	12.0860196030
H28	2.1371147662	-0.1514939634	12.2593541005
H29	2.7421541001	1.2912024947	10.3253958270
H30	-1.0799207199	-1.8896368177	9.9920019911
C31	-0.6558958480	-0.4211386462	7.6287044316
H32	-1.4491534816	-1.1716772417	7.6453897691
P33	1.3626120428	1.4272905414	7.5639186803
C34	4.9901853905	3.1829921148	4.2080076252
C35	5.5572264373	2.7519314468	5.4079899931
C36	4.7528522030	2.5426753052	6.5256896820
C37	3.3818959398	2.7778526234	6.4341514529
C38	2.8106760298	3.2269432630	5.2444899205
C39	3.6189958259	3.4195536075	4.1253424213
H40	5.6193566309	3.3363051527	3.3370745917
H41	6.6249357660	2.5681394816	5.4710592639
H42	5.1745462841	2.1839401553	7.4606257932
H43	1.7392110500	3.4079808646	5.1901804714
H44	3.1776486127	3.7560958911	3.1929077609
N45	2.5618880674	2.5476624569	7.5976841102
C46	2.5398945659	3.6161009698	8.6167271114
H47	2.3195922521	4.5772378318	8.1430570372
H48	1.7753761113	3.4064752486	9.3702065363
H49	3.5151755060	3.6727221440	9.1071630142

13-F^-

E(M06-2X/6-311+G**) = -1459.337765800

H(M06-2X/6-31+G*) = -1458.672840

C1	0.0455062443	-1.5880972756	6.3941772201
C2	0.0550580587	-1.5702815301	4.9987937871
C3	0.3134663226	-0.3800128196	4.3192590198
C4	0.5743835633	0.7899969498	5.0333155770
C5	0.5509962516	0.7764169878	6.4247619989
C6	1.9024523510	1.4845241525	8.8058835714
C7	3.0371395266	2.0594768493	9.3714763299
C8	3.7521619197	1.3843799294	10.3617607235
C9	3.3486495464	0.1139133709	10.7688625656
C10	2.2206729484	-0.4738526303	10.1951068786
C11	1.4908100883	0.2097792789	9.2247603702
C12	0.2830965825	-0.4160747067	7.1097717166
H13	-0.1578807191	-2.5139219889	6.9290910924
H14	-0.1390027319	-2.4848802373	4.4439136519
H15	0.3245986194	-0.3660937853	3.2322292726
H16	0.8113676759	1.7175039125	4.5183271747
H17	3.3693441714	3.0342654528	9.0255837958
H18	4.6319868679	1.8442819340	10.8046766734
H19	3.9098841662	-0.4201576780	11.5315111213
H20	1.8994246203	-1.4650061006	10.5105139754
C21	-2.9813852193	1.2717601247	9.9984888177
C22	-2.8090354024	2.5683567268	9.5192627487
C23	-1.6800916871	2.8996104410	8.7624307724
C24	-0.7066579781	1.9433075750	8.4775682474
C25	-0.8959387038	0.6438728031	8.9702655863
C26	-2.0161061776	0.3010474042	9.7209437957
H27	-3.8605307510	1.0139850152	10.5845895206

H28	-3.5587275016	3.3274204657	9.7326857705
H29	-1.5332305620	3.9029209384	8.3739661076
H30	-2.1362752770	-0.7172345934	10.0883815655
C31	0.2070931661	-0.3469981317	8.6275795812
H32	-0.0084415049	-1.3373381822	9.0444299021
N33	0.4623283784	3.7859940185	7.1198700818
P34	0.8984272180	2.2748516324	7.4518978952
F35	2.4277906015	2.3733990954	6.5658371378
C36	2.3584788608	7.0970514294	5.2999990755
C37	1.0166894451	6.7874789983	5.0687561691
C38	0.4324487145	5.6716468159	5.6574943314
C39	1.1570773586	4.8024491963	6.5089105324
C40	2.5148614197	5.1371173047	6.7285842994
C41	3.0935616999	6.2547131178	6.1374576664
H42	2.8181705257	7.9692285369	4.8424423804
H43	0.4162222573	7.4237683067	4.4206257787
H44	-0.6142091311	5.4360502888	5.4806646409
H45	3.1134009625	4.4919224150	7.3618467793
H46	4.1420886003	6.4715125864	6.3349108859

13-He$_8$-ring complex at 1.7 Å

E(BP86/6-31G*) = -1382.719802199

He1	2.0198000003	1.8632999998	11.4447000022
He2	6.2280000189	3.2546000137	9.1307000205
He3	4.8860000155	0.1784999892	10.2418000345
He4	3.3618000000	4.9395000000	10.3336000000
He5	3.1955000045	0.3896000202	11.1133999710

He6	5.0726000000	4.7344000000	9.5021000000
He7	6.1503999662	1.3673999954	9.4371999653
He8	2.0973999996	3.7504999999	11.1381999991
X9	4.1239000000	2.5590000000	10.2877000000
C10	1.5613422447	0.0073481338	4.0899878988
C11	0.8670536389	1.1176232863	3.5811252195
C12	0.8434324748	2.3139602842	4.3063020261
C13	1.5087530639	2.4160792285	5.5420699192
C14	2.2034251128	1.3098025141	6.0565742126
C15	4.6806634836	0.4719818320	6.8627551357
C16	5.9445315091	1.0751525458	6.8816807612
C17	7.0038416865	0.4948341796	6.1641743869
C18	6.7945823354	-0.6771318264	5.4227742946
C19	5.5136053207	-1.2506974981	5.3558578151
C20	4.4513989763	-0.6677273217	6.0595345867
C21	2.2279036169	0.0939893758	5.3178048240
H22	1.5854405183	-0.9345540856	3.5278848616
H23	0.3473328546	1.0422776201	2.6190814440
H24	0.3049527998	3.1852583165	3.9166941895
H25	1.4762748648	3.3583308262	6.0897721582
H26	6.0948482425	1.9983690288	7.4432661486
H27	7.9939574717	0.9642754082	6.1824295427
H28	7.6241666322	-1.1332428644	4.8704244121
H29	5.3357251083	-2.1376666097	4.7351026209
C30	0.9953124923	-2.8135967297	8.7087218791
C31	0.8847395407	-1.7463828272	9.6123701637
C32	1.5398528188	-0.5299219793	9.3550271825
C33	2.3178113668	-0.3902836992	8.1983476461
C34	2.3624284116	-1.4355241896	7.2472465934
C35	1.7181741220	-2.6510031122	7.5144326386

H36	0.4920272773	-3.7647185611	8.9158767946
H37	0.2820287584	-1.8559339030	10.5211098945
H38	1.4364814666	0.3114901419	10.0416881610
H39	1.7587544507	-3.4623801919	6.7770657632
C40	2.9990311443	-1.1063874490	5.8998512973
H41	2.9271058060	-1.9691159365	5.2162423338
P42	3.1655267422	1.1718468778	7.6700063169
N43	3.3659999949	2.3453999819	8.7810000074
C44	1.4858077817	5.9414891774	7.3815818965
C45	0.7784906085	5.0316850060	8.1855062641
C46	1.3938587529	3.8562898754	8.6387811364
C47	2.7367798230	3.5541684921	8.3073757754
C48	3.4337537095	4.4821806527	7.4968452109
C49	2.8184057908	5.6566648049	7.0403914518
H50	1.0039325742	6.8583738325	7.0234344087
H51	-0.2664606227	5.2318945673	8.4527100252
H52	0.8337086710	3.1397993191	9.2489742818
H53	4.4696559779	4.2593426700	7.2184705695
H54	3.3829595537	6.3502132714	6.4051094702

13-He_8-ring complex at 2.2 Å

E(BP86/6-31G*) = -1382.74013556

He1	2.0198000000	1.8633000000	11.4447000000
He2	6.2280000007	3.2546000002	9.1307000013
He3	4.8860000006	0.1785000002	10.2418000012
He4	3.3618000000	4.9395000000	10.3336000000
He5	3.1955000000	0.3896000000	11.1134000000

He6	5.0726000000	4.7344000000	9.5021000000
He7	6.1503999990	1.3673999998	9.4371999981
He8	2.0974000000	3.7505000000	11.1382000000
X9	4.1239000000	2.5590000000	10.2877000000
C10	-0.2860143289	0.1971526056	4.6092299347
C11	0.0578823596	1.0808013374	3.5711373653
C12	1.0067705395	2.0881750240	3.7887453289
C13	1.6196748941	2.2282895682	5.0470996157
C14	1.2723788844	1.3508306965	6.0849812752
C15	2.3726826041	-0.4651867060	7.8248836117
C16	3.6487821553	-0.9878606610	8.0586457907
C17	3.8476706155	-2.3769440472	7.9826323570
C18	2.7779672895	-3.2243778217	7.6579215066
C19	1.5079802492	-2.6911639090	7.3752212958
C20	1.3018208160	-1.3075992220	7.4471487188
C21	0.3156699229	0.3244591015	5.8668830044
H22	-1.0244871383	-0.5958192363	4.4372477178
H23	-0.4181344978	0.9762409437	2.5893953680
H24	1.2767796657	2.7745430081	2.9783732021
H25	2.3602741817	3.0144531198	5.2135999015
H26	4.4722598118	-0.3056342499	8.2794077235
H27	4.8425147758	-2.7963102914	8.1705405467
H28	2.9350576779	-4.3076847207	7.6018958050
H29	0.6834154840	-3.3529587162	7.0826547305
C30	-2.2404334238	0.9669808088	9.7585240497
C31	-1.4022071020	2.0009881671	10.2011135157
C32	-0.1160650431	2.1465933409	9.6524539842
C33	0.3218591787	1.2534621932	8.6672510254
C34	-0.5326378587	0.2301101322	8.1961294860
C35	-1.8105453934	0.0848283407	8.7513124673

H36	-3.2414274900	0.8505360910	10.1894979171
H37	-1.7479125639	2.6970035734	10.9735416357
H38	0.5442721646	2.9498025659	9.9866795829
H39	-2.4770911631	-0.7085699412	8.3907491885
C40	-0.0057398545	-0.6210314710	7.0392057385
H41	-0.7566773867	-1.3691447107	6.7323290639
P42	1.9660312897	1.3239843400	7.8119670414
N43	3.1431999997	2.2825999998	8.3378999993
C44	3.8191700825	5.8783810994	6.1348488209
C45	2.6356041888	5.7233717785	6.8740921821
C46	2.4047348483	4.5525067519	7.6104830158
C47	3.3458565069	3.4932011090	7.6162908337
C48	4.5375472503	3.6678900947	6.8713871718
C49	4.7689597292	4.8424125994	6.1428676187
H50	3.9999486439	6.7939454064	5.5603785232
H51	1.8824738395	6.5209434971	6.8793205353
H52	1.4774701871	4.4385963370	8.1851614406
H53	5.2675868059	2.8518968019	6.8639158055
H54	5.6972831898	4.9454148818	5.5674487932

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E(M06-2X/6-311+G**) = -1595.25369039637

H(M06-2X/6-31+G*) = -1594.380635

E(BP86/6-31G*) = -1595.46443103189

C1	-2.6139000045	0.2922897904	7.1843119443
C2	-3.3305455994	1.3502755445	6.6172090842
C3	-2.6823026720	2.5227328237	6.2358198784
C4	-1.3016946564	2.6464593454	6.4108382020

C5	-0.5922252011	1.5881327908	6.9626891070
C6	1.5843918841	-0.0569330084	6.5609442894
C7	2.6169195900	-0.3340169159	5.6688013904
C8	2.7814486961	-1.6429574630	5.2082359524
C9	1.9242342904	-2.6508243127	5.6409056996
C10	0.8935888706	-2.3689798499	6.5415616285
C11	0.7201626929	-1.0710629481	7.0060655874
C12	-1.2406941288	0.4100338559	7.3625298735
H13	-3.1277146003	-0.6164058554	7.4887240787
H14	-4.4037968675	1.2566510428	6.4794771622
H15	-3.2497183788	3.3420228617	5.8048478111
H16	-0.7778520957	3.5559459838	6.1295826432
H17	3.2862692990	0.4559924594	5.3375404161
H18	3.5827072424	-1.8716889306	4.5123230245
H19	2.0573697530	-3.6663894494	5.2798000152
H20	0.2307841037	-3.1616414422	6.8803459023
C21	0.7798968653	0.0699211397	11.5910097963
C22	1.5720112321	1.1955117255	11.3794730940
C23	1.7393805331	1.7009505801	10.0877347640
C24	1.1073517282	1.0664521377	9.0268689639
C25	0.3005401494	-0.0638853865	9.2334137307
C26	0.1411087556	-0.5624793628	10.5204344891
H27	0.6531949532	-0.3207366578	12.5964441595
H28	2.0596756743	1.6814598459	12.2190624429
H29	2.3512712440	2.5795201473	9.9022107220
H30	-0.4793251371	-1.4385748796	10.6930833016
C31	-0.3672628782	-0.6689288004	7.9991616153
H32	-0.9705819674	-1.5378392096	8.2773284484
P33	1.2079229538	1.5801996852	7.2791466867
N34	2.0375549085	2.8525085311	6.9409081439

C35	5.2404128548	3.5225192465	4.2809115632
C36	5.4356512902	3.5573183201	5.6577246339
C37	4.3820947031	3.3272499288	6.5429897752
C38	3.0900254285	3.0526770456	6.0320699620
C39	2.8817268262	3.0441652512	4.6301157536
C40	3.9671490771	3.2700260830	3.7808151507
H41	6.0707591382	3.6982672517	3.6034100134
H42	6.4276230498	3.7648517561	6.0495863267
H43	3.8148163135	3.2542861961	2.7052391009
C44	4.6061917139	3.3084818835	8.0427601900
H45	3.6761754792	3.6696271798	8.4957558367
C46	1.4875651475	2.8604753392	4.0572391658
H47	0.9188683176	2.2101088069	4.7310223793
C48	4.8446445545	1.8678122791	8.5183963853
H49	4.9236130623	1.8169134615	9.6114539832
H50	4.0326645131	1.2009851152	8.2078920134
H51	5.7770811544	1.4806070726	8.0900452673
C52	5.7438651378	4.2153060175	8.5153367681
H53	5.7515186743	4.2626547799	9.6098485179
H54	6.7242470582	3.8385499877	8.2021197149
H55	5.6306920983	5.2339183753	8.1299590666
C56	0.7749417648	4.2193433218	4.0143975034
H57	-0.2708459171	4.1075105737	3.7023490113
H58	0.8034879219	4.7031501050	4.9962057194
H59	1.2775720537	4.8819396971	3.2999243583
C60	1.4560593152	2.1888774062	2.6830928775
H61	0.4207333705	1.9668043273	2.4033012260
H62	1.8729155900	2.8334393066	1.9015044245
H63	2.0176409374	1.2483176916	2.6871483904

14-H$^+$

E(M06-2X/6-311+G**) = -1595.65930718011

H(M06-2X/6-31+G*) = -1594.770122

C1	-2.0714831435	1.9366203158	7.8953043020
C2	-2.2289682890	3.2372188363	7.4122829420
C3	-1.1684805854	3.8995121677	6.8022173744
C4	0.0713151580	3.2740771824	6.6631497541
C5	0.2209593507	1.9750179394	7.1476699042
C6	0.9837058132	-0.6149875969	6.4149541927
C7	1.4907167866	-1.3478649317	5.3476717365
C8	0.8194789331	-2.5076348897	4.9571190342
C9	-0.3329954588	-2.9071347662	5.6301387036
C10	-0.8329499710	-2.1651903536	6.7043201455
C11	-0.1719818906	-1.0125201283	7.1075856305
C12	-0.8474692792	1.2931239002	7.7686215946
H13	-2.9039235222	1.4258629200	8.3710833737
H14	-3.1886002101	3.7335220456	7.5155780079
H15	-1.2990547652	4.9101327510	6.4300043935
H16	0.8917350508	3.7989513134	6.1867154000
H17	2.3891977689	-1.0267038622	4.8261730408
H18	1.1969426723	-3.0968628779	4.1280644695
H19	-0.8504687417	-3.8090275676	5.3191071916
H20	-1.7310493483	-2.4897703020	7.2224163368
C21	1.5207288786	-0.4954944297	11.4633443045
C22	2.7441870869	-0.0063020381	11.0115062146

C23	2.8744436354	0.4479824810	9.6982316929
C24	1.7624906209	0.3957466962	8.8652610499
C25	0.5262284631	-0.1048964162	9.3055333439
C26	0.4098130559	-0.5473313661	10.6164411966
H27	1.4272929144	-0.8444521743	12.4867982141
H28	3.5980520528	0.0231180074	11.6802072541
H29	3.8245002841	0.8344671443	9.3373416802
H30	-0.5377553209	-0.9341024196	10.9800858066
C31	-0.6093623275	-0.1311827816	8.2797510623
H32	-1.5231754530	-0.5231114491	8.7316161379
P33	1.6607344789	0.8910002581	7.1361156352
C34	3.4494867028	5.3063492053	4.7530013965
C35	3.7212265785	5.1193074585	6.1040795244
C36	3.5935590407	3.8591056568	6.6936764119
C37	3.1875843907	2.7953631654	5.8682735053
C38	2.8912965851	2.9597657645	4.5034494172
C39	3.0354758826	4.2397291978	3.9623595511
H40	3.5526804005	6.2940659441	4.3143910253
H41	4.0265490678	5.9673642794	6.7071711350
H42	2.8122449494	4.4095304153	2.9146816359
N43	3.0338446421	1.4781692115	6.4603372869
H44	3.8336645777	0.8505100219	6.4246266750
C45	3.8912581540	3.6438314107	8.1684831649
H46	3.1426830400	2.9416416463	8.5575378376
C47	2.4405485102	1.7879019917	3.6473780791
H48	1.7690556214	1.1706937756	4.2580687130
C49	3.6465300559	0.9277792672	3.2422929323
H50	3.3231361665	0.0562417929	2.6626692897
H51	4.3329592590	1.5105515248	2.6190538419
H52	4.2150128318	0.5718340040	4.1087286717

C53	1.6489592677	2.2022630586	2.4059934090
H54	1.2334540955	1.3130815792	1.9230650227
H55	0.8190007557	2.8694456114	2.6589459240
H56	2.2833529777	2.7041274717	1.6682610120
C57	5.2798950810	3.0124285998	8.3461877380
H58	5.4839563661	2.8186980435	9.4049762352
H59	5.3817627832	2.0685391453	7.7990256873
H60	6.0535293895	3.6922309905	7.9739321266
C61	3.7797215503	4.9162702140	9.0101246361
H62	3.8593676263	4.6615325834	10.0709189968
H63	4.5850858964	5.6233900532	8.7860903089
H64	2.8217621643	5.4222278722	8.8540278722

14-Me$^+$

E(M06-2X/6-311+G**) = -1634.95829708235

H(M06-2X/6-31+G*) = -1634.030722

C1	-2.6231387721	0.7401905653	7.4772738917
C2	-3.2572088652	1.9726100977	7.2974208694
C3	-2.5166981692	3.1454913227	7.1730473822
C4	-1.1228734557	3.1016129816	7.2216659821
C5	-0.4989657296	1.8712314521	7.3972894186
C6	1.4563305112	0.2210441457	6.2684223273
C7	2.3363554179	0.1064681755	5.1913864558
C8	2.2659451759	-1.0276966722	4.3828957310
C9	1.3342094634	-2.0269811141	4.6457496961
C10	0.4549070256	-1.9074651555	5.7223349014
C11	0.5064472158	-0.7859730555	6.5408999295

C12	-1.2367509988	0.6836917827	7.5322765404
H13	-3.2107158103	-0.1683759655	7.5754012769
H14	-4.3409524894	2.0148166812	7.2572664912
H15	-3.0218552880	4.0962060255	7.0385547215
H16	-0.5428307768	4.0151842599	7.1276224651
H17	3.0679981753	0.8745074813	4.9708377386
H18	2.9471130890	-1.1235457393	3.5438976253
H19	1.2882639295	-2.9057115364	4.0104808448
H20	-0.2724317100	-2.6888012262	5.9239348454
C21	1.0892430690	-1.0791809381	11.2276241585
C22	1.9894451055	-0.0172637573	11.2625606554
C23	2.1112481364	0.8327663262	10.1627663253
C24	1.3216384259	0.5967708082	9.0416819296
C25	0.3987521885	-0.4618788409	9.0040746707
C26	0.2906305546	-1.3039570299	10.1031399976
H27	1.0016124183	-1.7379317882	12.0856657250
H28	2.5973327618	0.1529657744	12.1449372276
H29	2.8075342609	1.6654075276	10.1942009625
H30	-0.4136388637	-2.1310912838	10.0889876654
C31	-0.4366467092	-0.6035917884	7.7317682873
H32	-1.1078077863	-1.4615293218	7.8104341384
P33	1.2721805419	1.5361431959	7.4986170900
C34	5.1623356842	2.9174300553	4.3331394515
C35	5.4774768870	2.3615352013	5.5685217218
C36	4.5505891566	2.3621297282	6.6141396857
C37	3.2850442445	2.9229267646	6.3651211780
C38	2.9628811987	3.5437365322	5.1441103851
C39	3.9237318240	3.5180528109	4.1304011695
H40	5.8921329882	2.8989819146	3.5295118354
H41	6.4573785322	1.9184942885	5.7219472472

H42	3.7005168159	3.9714733160	3.1690971065
N43	2.2656809377	2.8358935321	7.3914093589
C44	2.1830927962	3.9274445968	8.3745753060
H45	1.9878222711	4.8735890781	7.8594868167
H46	1.3756512099	3.7400621993	9.0895866553
H47	3.1293611043	4.0107122270	8.9195623929
C48	4.9219330686	1.7536695684	7.9553564842
H49	4.1409090817	2.0279099773	8.6691673431
C50	1.6152395424	4.2008813876	4.8981526203
H51	1.1313670697	4.3332955115	5.8700099184
C52	0.7070148372	3.3059945716	4.0441036303
H53	-0.2666076074	3.7839579999	3.8920715725
H54	1.1563074980	3.1295004507	3.0601619556
H55	0.5345113511	2.3294448142	4.5111970578
C56	1.7602810221	5.5918284679	4.2698291563
H57	0.7848543748	6.0864181986	4.2273678835
H58	2.4417522329	6.2232782157	4.8484140550
H59	2.1401518276	5.5351125429	3.2449562277
C60	4.9715305211	0.2218411449	7.8855164042
H61	5.2298876969	-0.1958211015	8.8643896156
H62	4.0107124970	-0.2063416299	7.5776192962
H63	5.7294573644	-0.1077167251	7.1658587121
C64	6.2429204331	2.3220382073	8.4869818360
H65	6.4295482391	1.9545450194	9.5009918778
H66	7.0906800859	2.0149598001	7.8669161311
H67	6.2241169088	3.4158779605	8.5144141418

14-F^-

E(M06-2X/6-311+G**) = -1695.16832747081

H(M06-2X/6-31+G*) = -1694.264138

C1	-0.4268628489	-1.1776824684	6.0300828785
C2	-0.4091181105	-0.9523182419	4.6530037488
C3	0.0492418643	0.2660006752	4.1515486257
C4	0.4947801632	1.2578467158	5.0257200472
C5	0.4487884307	1.0465963407	6.4021741624
C6	1.9313105151	1.1694123443	8.7966572170
C7	3.1573609255	1.4459109010	9.3979894474
C8	3.7667753197	0.5110179902	10.2367049108
C9	3.1652128646	-0.7255986454	10.4579054898
C10	1.9450335616	-1.0179930282	9.8486702005
C11	1.3226816843	-0.0760868912	9.0320999494
C12	-0.0061196576	-0.1782304655	6.9058903035
H13	-0.7755342348	-2.1302265635	6.4250989844
H14	-0.7472741468	-1.7298862998	3.9725896151
H15	0.0744543605	0.4384928797	3.0785025263
H16	0.8984255321	2.1942355151	4.6464922876
H17	3.6512237318	2.3922618625	9.2019263612
H18	4.7195317113	0.7453928943	10.7047733662
H19	3.6418914355	-1.4611851867	11.1009205245
H20	1.4665464722	-1.9813214895	10.0162383731
C21	-2.9175433508	1.5105701330	10.1520149509
C22	-2.5410264985	2.8261876572	9.8914069159
C23	-1.3827602476	3.0979049549	9.1556235925
C24	-0.5811289295	2.0632366123	8.6758648292
C25	-0.9713245420	0.7461802164	8.9571549180
C26	-2.1250870277	0.4615251173	9.6806187581

H27	-3.8214743106	1.2987592523	10.7183202811
H28	-3.1537363032	3.6469859582	10.2578218135
H29	-1.0800382007	4.1174065076	8.9370666081
H30	-2.4050654420	-0.5726215605	9.8764858834
C31	-0.0457379678	-0.3312902989	8.4174296499
H32	-0.4029414461	-1.3306811665	8.6905230633
N33	0.8009159683	3.9000944429	7.5284715315
P34	1.0212588026	2.3124089095	7.6251623595
F35	2.5401157854	2.3554813941	6.7124490473
C36	2.3217212323	6.7559479435	4.8244095601
C37	1.0951529907	6.1363966066	4.6027860769
C38	0.6020278261	5.1692221157	5.4797942796
C39	1.3612414835	4.7886360467	6.6226391845
C40	2.6042514671	5.4409229986	6.8510605201
C41	3.0601737925	6.4050574771	5.9524987948
H42	2.6968603419	7.5040678183	4.1303264102
H43	0.5086531223	6.4172998253	3.7301542102
H44	4.0173697208	6.8907121021	6.1279361892
C45	-0.7882538166	4.5868628135	5.2895593183
H46	-0.7940827277	3.5892950335	5.7385734401
C47	3.3913151031	5.0832379703	8.0949283776
H48	3.3266251086	3.9962722872	8.1750726228
C49	-1.8059447790	5.4272094081	6.0730916408
H50	-2.8067979834	4.9787666139	6.0289065732
H51	-1.5027863401	5.4968597187	7.1216422320
H52	-1.8597232559	6.4428705917	5.6592727594
C53	-1.2178267623	4.4487435673	3.8280250345
H54	-2.1592696968	3.8902974440	3.7658107557
H55	-1.3841381393	5.4252556489	3.3565079920
H56	-0.4648493812	3.9137052595	3.2381484135

C57	4.8729489390	5.4530180545	8.0362655102
H58	5.3932613005	5.0438236365	8.9110294570
H59	5.3508294196	5.0515708651	7.1359124041
H60	5.0228075089	6.5404403549	8.0492170987
C61	2.7380127726	5.6896479698	9.3434347703
H62	3.2537741609	5.3575005760	10.2544435835
H63	2.7862238223	6.7858066022	9.3014726147
H64	1.6901243916	5.3832345165	9.4058816394

14-He$_8$-ring complex at 1.7 Å

E(BP86/6-31G*) = -1618.5641793224

He1	2.0198000010#	1.8633000004#	11.4447000030#
He2	6.2280000000#	3.2546000000#	9.1307000000#
He3	4.8860000000#	0.1785000000#	10.2418000000#
He4	3.3617999650#	4.9394999934#	10.3335999352#
He5	3.1954999991#	0.3895999997#	11.1133999981#
He6	5.0726000241#	4.7344000068#	9.5021000479#
He7	6.1504000000#	1.3674000000#	9.4372000000#
He8	2.0974000279#	3.7505000031#	11.1382000384#
X9	4.1239000000#	2.5590000000#	10.2877000000#
C10	1.8287327294	-0.0116105775	3.9743961854
C11	1.0691843411	1.0606366744	3.4826316987
C12	0.9520499087	2.2298123136	4.2423761576
C13	1.5882354753	2.3394072108	5.4914467957
C14	2.3535298259	1.2701727830	5.9929919022
C15	4.8817119813	0.5491746926	6.8371655208
C16	6.1454301330	1.1496673459	6.9286308624
C17	7.2425597638	0.6083768304	6.2395847120

C18	7.0847897168	-0.5334228036	5.4437168137
C19	5.8147694182	-1.1150556284	5.3075653558
C20	4.7166603424	-0.5704761698	5.9874435412
C21	2.4673240355	0.0845525406	5.2173545587
H22	1.9276466938	-0.9343385652	3.3894613169
H23	0.5719525026	0.9783649041	2.5094906675
H24	0.3613499502	3.0744995325	3.8707138880
H25	1.4806379076	3.2620842124	6.0612063978
H26	6.2817496745	2.0472056664	7.5263624768
H27	8.2234771331	1.0890289264	6.3256705473
H28	7.9422845934	-0.9598901699	4.9108582498
H29	5.6696810879	-1.9853305309	4.6553190745
C30	1.4702916394	-3.0629709154	8.5048165283
C31	1.3021672125	-2.0617008506	9.4699632517
C32	1.8425664495	-0.7814971712	9.2640095184
C33	2.5651108140	-0.4963100350	8.0969257732
C34	2.6789131819	-1.4930859341	7.0988302461
C35	2.1469643090	-2.7719412444	7.3104416848
H36	1.0545687847	-4.0637477741	8.6678956314
H37	0.7426979311	-2.2698045093	10.3888977141
H38	1.6812115280	-0.0044470349	10.0077667416
H39	2.2458546941	-3.5354071050	6.5288664442
C40	3.2985215109	-1.0780195249	5.7730750550
H41	3.2936003313	-1.9227640184	5.0629312948
P42	3.2965252981	1.1639500363	7.6328621640
N43	3.3659999829#	2.3453999966#	8.7809999774#
C44	1.0881350043	5.8064140910	7.4481518375
C45	0.4808830668	4.7880435271	8.1854481876
C46	1.1873261499	3.6430997354	8.6038664691
C47	2.5873606795	3.5041739369	8.2910887027

C48	3.1927001276	4.5394619038	7.4901730870
C49	2.4328734446	5.6608466293	7.1008455676
H50	0.5195515632	6.6896048753	7.1350432695
H51	-0.5844273344	4.8677895563	8.4330791497
H52	2.9137144218	6.4343379428	6.4903966033
C53	0.3626132106	2.5524727147	9.2956454613
H54	1.0789279865	1.8405936853	9.7234981006
C55	4.6228843631	4.4704597146	6.9411284481
H56	5.1463516218	3.6978492115	7.5174812580
C57	-0.5441212450	3.0779514882	10.4341582781
H58	-0.9814300007	2.2280176619	10.9902941972
H59	-0.0029605195	3.7146320086	11.1507521665
H60	-1.3912145925	3.6672543898	10.0373744064
C61	-0.5215946654	1.7786824402	8.2869041979
H62	-1.1038711215	0.9950332633	8.8072337615
H63	-1.2388368025	2.4604450619	7.7930556034
H64	0.0708362561	1.2896271791	7.4969317181
C65	5.4039541001	5.8014291524	7.0746220673
H66	6.4804465140	5.6283109247	6.8903998947
H67	5.0691679892	6.5410630527	6.3241139958
H68	5.2949001495	6.2642076551	8.0678095259
C69	4.6558491785	4.0465404227	5.4515880740
H70	5.6986668542	4.0230579420	5.0831351121
H71	4.2178161408	3.0501982170	5.2834464435
H72	4.0940727364	4.7678076819	4.8292143702

14-He$_8$-ring complex at 2.2 Å

E(BP86/6-31G*) = -1618.5938307245

He1	2.0197996364#	1.8632999911#	11.4446998530#
He2	6.2280001646#	3.2545998536#	9.1307001817#
He3	4.8860000000#	0.1785000000#	10.2418000000#
He4	3.3617997507#	4.9394998884#	10.3336001313#
He5	3.1955000751#	0.3896000234#	11.1134001628#
He6	5.0725998862#	4.7344000042#	9.5020998031#
He7	6.1503999231#	1.3674001818#	9.4371998713#
He8	2.0974005926#	3.7504999244#	11.1381998484#
X9	4.1239000000#	2.5590000000#	10.2877000000#
C10	0.9555648903	-0.2806852298	3.9900839196
C11	0.6009727237	0.8816397490	3.2862232569
C12	0.8829752702	2.1413230693	3.8296628667
C13	1.5195019575	2.2530443648	5.0781952636
C14	1.8759988986	1.0922647183	5.7871798819
C15	4.0250321183	-0.2325062551	6.9284907548
C16	5.4068802252	-0.0990420679	7.1086937660
C17	6.2766484907	-1.1030629199	6.6494113751
C18	5.7655347333	-2.2375138732	6.0048986343
C19	4.3812894970	-2.3676954078	5.8039498028
C20	3.5106415731	-1.3694059641	6.2594369577
C21	1.5909008038	-0.1832096070	5.2346511718
H22	0.7376003920	-1.2702934599	3.5694888302
H23	0.1042855176	0.7988994828	2.3126782321
H24	0.6089272440	3.0514411394	3.2845645768
H25	1.7325130618	3.2410230571	5.4902735826
H26	5.8067148032	0.7889447892	7.5965060046
H27	7.3571314516	-0.9925425717	6.7953920506
H28	6.4438058787	-3.0210298077	5.6481756413
H29	3.9776541835	-3.2460004706	5.2849943707

C30	-0.2229465075	-2.2223639237	9.0827561409
C31	0.0169026002	-1.0915586034	9.8755236225
C32	0.9042803258	-0.0949246164	9.4345600209
C33	1.5540108386	-0.2350913406	8.2027784334
C34	1.2998256396	-1.3681231046	7.3942050277
C35	0.4148152847	-2.3586446101	7.8382068517
H36	-0.9144711234	-2.9995385566	9.4277949827
H37	-0.4886611724	-0.9794023264	10.8413316672
H38	1.0866650187	0.7907731106	10.0425183486
H39	0.2180381571	-3.2351725763	7.2084365716
C40	2.0001695058	-1.4221871013	6.0381413606
H41	1.7205368713	-2.3398152155	5.4935823489
P42	2.7249431131	0.9949916294	7.4522011449
N43	3.1431999712#	2.2826001332#	8.3379001484#
C44	2.3292396865	6.1146398282	6.5609577702
C45	1.3919161920	5.5015154417	7.3981510800
C46	1.6369063699	4.2504474431	7.9951989006
C47	2.8765133270	3.5733934768	7.7373527897
C48	3.8433055128	4.2152823655	6.8930687429
C49	3.5444326929	5.4666574968	6.3214383611
H50	2.1152615258	7.0869307607	6.1016226305
H51	0.4348486980	6.0018870455	7.5887131341
H52	4.2836654183	5.9385476134	5.6627117081
C53	0.5312090869	3.6345014811	8.8555882932
H54	1.0057496798	2.8435334471	9.4580348713
C55	5.1758129577	3.5597307596	6.5277661585
H56	5.3262635202	2.7392116320	7.2466996803
C57	-0.5706384190	2.9745716074	7.9926947825
H58	-1.3550095919	2.5306152666	8.6344072196
H59	-1.0526571323	3.7251497290	7.3386116326

H60	-0.1733131606	2.1755222034	7.3451704793
C61	-0.1248079631	4.6527325492	9.8169366670
H62	-0.7570802087	4.1270503117	10.5563718847
H63	0.6235150615	5.2481637686	10.3647753056
H64	-0.7829023889	5.3573868432	9.2756607403
C65	6.3795678008	4.5233568115	6.6355950350
H66	7.3263890066	3.9653771669	6.5115238965
H67	6.3559350817	5.2945111672	5.8436809397
H68	6.4110055776	5.0421408430	7.6070270475
C69	5.1421400838	2.9484804349	5.1066499302
H70	6.1054283828	2.4593371533	4.8684764599
H71	4.3447062222	2.1950817216	4.9947336798
H72	4.9656951142	3.7353941259	4.3494978142

Cmpd B

E(M06-2X/6-311+G**) = -1569.61962981991

H(M06-2X/6-31+G*) = -1568.74416

C1	7.9857037479	7.8896442566	2.3160890820
C2	6.8953144760	8.7733649570	2.5177181593
C3	5.6611830086	8.4730174097	1.9418225479
H4	4.8226605943	9.1484316552	2.0821679292
C5	5.4849748954	7.3207686294	1.1821797353
H6	4.5180975432	7.0991886253	0.7399300742
C7	6.5558936940	6.4552166384	0.9922553792
H8	6.4086326114	5.5592200533	0.3975452501
C9	7.8126821348	6.7137636130	1.5466178442
C10	8.9589614624	5.7303542060	1.3727283163
H11	9.8560741057	6.2979162352	1.1039513981

C12	9.2502419735	4.9968723193	2.6893212913
H13	9.4204570832	5.7001877491	3.5090083135
H14	10.1380444830	4.3621352801	2.5871623626
H15	8.3989597175	4.3593213698	2.9554799826
C16	8.7580497710	4.7238969963	0.2396746776
H17	7.9528702291	4.0148032881	0.4640684651
H18	9.6766660830	4.1445446116	0.1009673957
H19	8.5265289837	5.2215948748	-0.7081670829
C20	7.0906381292	10.0175776943	3.3682344754
H21	8.0559763378	10.4552956745	3.0770955683
C22	6.0246014089	11.0932287765	3.1566674550
H23	5.9119367704	11.3534180204	2.0983977187
H24	6.3008465799	12.0011768846	3.7032813407
H25	5.0470925681	10.7727859360	3.5345578990
C26	7.1841391247	9.6483695167	4.8559958619
H27	6.2298077126	9.2299382701	5.1966446134
H28	7.4006705791	10.5365336004	5.4628748480
H29	7.9691775390	8.9067145577	5.0245748493
C30	9.4974654489	9.7743338535	0.1709430819
H31	9.9227146002	10.5605722597	-0.4612857175
H32	8.9366869604	10.2435112723	0.9816778987
H33	8.8032545103	9.1614143189	-0.4169835720
C34	11.3676305727	8.1713477576	-0.0952299456
C35	11.4114300452	8.1974830045	-1.4832124343
H36	10.8012266658	8.8980040772	-2.0442286209
C37	12.2677476923	7.3080489474	-2.1419910930
H38	12.3168364083	7.3242548340	-3.2262263184
C39	13.0448548086	6.4039650507	-1.4265029074
H40	13.6976257492	5.7137977722	-1.9507789244
C41	12.9785553969	6.3594985918	-0.0280982969

H42	13.5535366798	5.6263008747	0.5251758781
C43	12.1482684343	7.2502822354	0.6304758158
C44	12.9727243734	7.5687263647	2.9580124539
C45	14.1307088020	6.8265180453	3.1154889137
H46	14.3221694385	5.9582959034	2.4964033348
C47	15.0458491902	7.2045493518	4.1056357250
H48	15.9583588726	6.6315289528	4.2334837743
C49	14.7849363475	8.2912064285	4.9321183557
H50	15.4953130729	8.5668302891	5.7051968379
C51	13.6105677901	9.0372839696	4.7856295641
H52	13.4087004390	9.8850911049	5.4322493262
C53	12.7160842855	8.6763497211	3.7869602729
C54	10.9077083906	10.2216249113	4.4508290032
H55	10.8207841973	9.7562259442	5.4396914014
H56	9.9089702789	10.4983026874	4.1141604525
H57	11.5260868290	11.1218642924	4.5236263784
N58	9.1967988862	8.2148732223	2.9500195990
N59	10.5616617082	8.9594074238	0.7322654950
N60	11.9235795922	7.3681964325	2.0257473856
N61	11.4928194570	9.2932976763	3.4997843329
P62	10.6050597215	8.4476306720	2.3473955839

Cmpd B-H$^+$

E(M06-2X/6-311+G**) = -1570.02159388208

H(M06-2X/6-31+G*) = -1569.129547

C1	8.0345123681	7.8272207068	2.4017393843
C2	6.9819481249	8.7632530218	2.4704296702

C3	5.8229847795	8.4913932837	1.7449989889
H4	4.9933703276	9.1894212167	1.7723471730
C5	5.7193965718	7.3373835391	0.9729772553
H6	4.8123635163	7.1447388763	0.4084623554
C7	6.7673273954	6.4286619139	0.9304102584
H8	6.6644109919	5.5244991885	0.3385106059
C9	7.9484262174	6.6444600064	1.6507465175
C10	9.0157928996	5.5620874005	1.6587019085
H11	9.9483823856	5.9736212795	2.0531903332
C12	8.5887631657	4.4368117360	2.6143731832
H13	8.4169566898	4.8152032042	3.6274319301
H14	9.3607465377	3.6624035710	2.6615465867
H15	7.6597892268	3.9708625241	2.2684657688
C16	9.3200743866	5.0047584871	0.2634468354
H17	8.4794407778	4.4271382253	-0.1339871714
H18	10.1807442421	4.3305742508	0.3159591594
H19	9.5563543763	5.8005257015	-0.4508583748
C20	7.0914491933	10.0090011891	3.3349475810
H21	8.1361761898	10.3460462565	3.2974126936
C22	6.2256528293	11.1734751514	2.8486307375
H23	6.3857936730	11.3835803040	1.7857707523
H24	6.4677866240	12.0770624123	3.4159750229
H25	5.1598813387	10.9753400588	2.9990685159
C26	6.7644200869	9.6796215577	4.7998850266
H27	5.7266520710	9.3414283701	4.8869341725
H28	6.8882626923	10.5647059096	5.4324685356
H29	7.3994348487	8.8821495207	5.2034188756
C30	9.3699234128	9.8506167722	0.4371268435
H31	9.8241931421	10.5573500912	-0.2625799894
H32	8.9563442972	10.4120002777	1.2763677549

H33	8.5609465329	9.2981246276	-0.0517561362
C34	11.1313581776	8.1266194326	0.0146118546
C35	11.0032020313	8.1194866963	-1.3657091492
H36	10.3233028240	8.7963603486	-1.8721780348
C37	11.7721085042	7.2029781975	-2.0894408157
H38	11.6891840498	7.1806907853	-3.1708294349
C39	12.6265240194	6.3146400166	-1.4424437402
H40	13.2034142425	5.6016563875	-2.0212943050
C41	12.7419622748	6.3172865936	-0.0487111133
H42	13.3813519664	5.6006239310	0.4530316493
C43	12.0012684387	7.2416667322	0.6675764851
C44	13.0833846175	7.6581011740	2.9173115679
C45	14.2955855068	6.9893448507	2.9164285503
H46	14.4828455530	6.1649193890	2.2396316672
C47	15.2794866662	7.4041059562	3.8186792842
H48	16.2369861419	6.8948647905	3.8281321911
C49	15.0426638360	8.4502083560	4.7052525656
H50	15.8160289428	8.7524309002	5.4030927024
C51	13.8165455841	9.1210846828	4.7127057118
H52	13.6351224848	9.9377068271	5.4037279482
C53	12.8489568800	8.7145158728	3.8076971079
C54	11.0685513343	10.3036246505	4.5664919193
H55	11.1239826649	9.9680482336	5.6064996301
H56	10.0319238719	10.5490832699	4.3287578474
H57	11.6813235728	11.2003555758	4.4397542605
N58	10.3942679038	8.9300621061	0.9197888071
N59	11.9518420707	7.4257102163	2.0813223815
N60	11.5392801659	9.2454642195	3.6785889874
P61	10.7019662774	8.4807774812	2.4780426864
N62	9.2475384354	8.1397351505	3.1348673086

H63	9.2095183586	8.0716441419	4.1499184375

Cmpd B-Me$^+$

E(M06-2X/6-311+G**) = -1609.3179033042

H(M06-2X/6-31+G*) = -1608.387123

C1	8.0717294547	7.8342562794	2.4559758318
C2	7.0173402891	8.7677486711	2.5209513112
C3	5.8640924212	8.5054445473	1.7785195183
H4	5.0353679378	9.2063193966	1.8132231905
C5	5.7617751072	7.3630408613	0.9937210667
H6	4.8612510415	7.1803562522	0.4157721337
C7	6.8044301524	6.4460696128	0.9636475686
H8	6.7029709382	5.5444803512	0.3675396195
C9	7.9746576218	6.6485264474	1.7022196220
C10	9.0226751360	5.5463725314	1.7258037906
H11	9.9545032608	5.9402530543	2.1408578192
C12	8.5586050556	4.4183137431	2.6616206156
H13	8.3712739894	4.7842698015	3.6761250053
H14	9.3177822086	3.6317168397	2.7158375503
H15	7.6299911604	3.9703018403	2.2920338380
C16	9.3399574853	4.9842581621	0.3346966731
H17	8.5004807648	4.4077257728	-0.0669005619
H18	10.1972958544	4.3067650208	0.3981291136
H19	9.5847060116	5.7749229685	-0.3815624421
C20	7.0645828271	10.0060291298	3.4014534919
H21	8.1097008367	10.1788240207	3.6868234411
C22	6.5604655221	11.2711298857	2.6945281371

H23	7.0418750358	11.4279123792	1.7241534624
H24	6.7523467821	12.1494295536	3.3186848069
H25	5.4807090020	11.2285245377	2.5231251391
C26	6.2505181481	9.7730668246	4.6850289492
H27	5.1896892180	9.6544640338	4.4398959712
H28	6.3460869893	10.6275158407	5.3629596048
H29	6.5660814986	8.8696978237	5.2155421414
C30	9.3598309490	9.8942724328	0.5027946402
H31	9.8176070327	10.5781663870	-0.2173761094
H32	9.0105899866	10.4746624887	1.3583268290
H33	8.5046113356	9.3807987390	0.0510122586
C34	11.0611424702	8.1149460572	0.0349087809
C35	10.8968352836	8.1013712755	-1.3412576304
H36	10.2028237770	8.7757442161	-1.8318197095
C37	11.6494948687	7.1839362874	-2.0813233629
H38	11.5387635799	7.1573358611	-3.1601107571
C39	12.5238272607	6.3013857446	-1.4535371343
H40	13.0890603409	5.5889280189	-2.0443868800
C41	12.6745680031	6.3098119948	-0.0629651798
H42	13.3309486077	5.5992350843	0.4256207422
C43	11.9490963621	7.2332613755	0.6691138268
C44	13.1027792946	7.6859476478	2.8722251641
C45	14.3134558498	7.0147849057	2.8569104988
H46	14.4778798869	6.1678453866	2.2020833161
C47	15.3253837968	7.4558748352	3.7150363922
H48	16.2822717161	6.9454251416	3.7113950589
C49	15.1166823619	8.5290328192	4.5759425413
H50	15.9110790908	8.8509191195	5.2406933748
C51	13.8918643539	9.2024735548	4.5996291941
H52	13.7318515318	10.0406523665	5.2699679777

C53	12.8979098326	8.7715294969	3.7350460654
C54	11.1420195840	10.3874094635	4.4898814567
H55	11.2055721760	10.0844371569	5.5398756120
H56	10.1059597814	10.6391576609	4.2566022911
H57	11.7619570134	11.2734573495	4.3269613296
N58	10.3581938006	8.9334677669	0.9527757053
N59	11.9424237759	7.4227328211	2.0844332706
N60	11.5878197661	9.3020865010	3.6268767675
P61	10.6982864956	8.4834767246	2.5027799475
N62	9.2801560970	8.1085210579	3.2222716190
C63	9.2415309011	7.8083041450	4.6688461701
H64	8.5538475082	6.9755499196	4.8227902643
H65	10.2307418936	7.5163028709	5.0299657709
H66	8.8894038974	8.6733106560	5.2394383985

Cmpd B-F^-

E(M06-2X/6-311+G**) = -1669.57031242086

H(M06-2X/6-31+G*) = -1668.662981

C1	8.5089829750	8.0025701643	2.0226132057
C2	7.3449697591	8.8205189219	1.9933981507
C3	6.2599168593	8.4606803529	1.1954534622
H4	5.3807318286	9.0999912060	1.1600459295
C5	6.2881409159	7.3019889032	0.4213187322
H6	5.4432088888	7.0410207736	-0.2109474793
C7	7.4096714136	6.4775604641	0.4763307438
H8	7.4238347029	5.5646920814	-0.1144151069
C9	8.5127335646	6.7949998878	1.2716060437

C10	9.6709342255	5.8245564390	1.4230340419
H11	10.5879536911	6.4034170482	1.5386343262
C12	9.4941256574	5.0263699578	2.7227742172
H13	9.4161209937	5.7098776432	3.5738041182
H14	10.3493802510	4.3593313079	2.8886645299
H15	8.5823380436	4.4166891473	2.6750277923
C16	9.8818131590	4.8931722619	0.2298154987
H17	9.0692977618	4.1612301277	0.1312068788
H18	10.8158511310	4.3347679642	0.3602120390
H19	9.9604557797	5.4585079031	-0.7054550203
C20	7.3266953713	10.0693313363	2.8565295655
H21	8.3329437410	10.5047693268	2.8086516763
C22	6.3283166795	11.1337015950	2.4008588686
H23	6.4642721878	11.3875243325	1.3430950727
H24	6.4603007147	12.0476735288	2.9916791531
H25	5.2915117912	10.8026902405	2.5391856785
C26	7.0714686776	9.6883117397	4.3221068310
H27	6.0638741749	9.2667068946	4.4320852905
H28	7.1493628040	10.5669612458	4.9763687669
H29	7.8012117062	8.9407696088	4.6466683842
C30	9.7161883326	9.7945508548	-0.0787733530
H31	10.1406413911	10.4204821679	-0.8781284434
H32	9.2373383568	10.4514878749	0.6491270484
H33	8.9459389435	9.1372822878	-0.5091378739
C34	11.5470962106	8.2107086906	-0.1570163000
C35	11.4496463285	7.8904606436	-1.5127211522
H36	10.6782788100	8.3469786190	-2.1252880345
C37	12.3345627528	6.9509722150	-2.0592520504
H38	12.2552143451	6.6968070402	-3.1132752431
C39	13.2867815020	6.3257493203	-1.2652695877

H40	13.9479277247	5.5749086907	-1.6880661878
C41	13.3979107447	6.6516679220	0.0988290666
H42	14.1120706579	6.1246595702	0.7192307160
C43	12.5606832300	7.6149009515	0.6395125077
C44	13.4564066397	8.0449983910	2.9307149014
C45	14.7775340459	7.6341270559	2.8460827902
H46	15.1875378197	7.2608614898	1.9168562494
C47	15.6079831477	7.7400066444	3.9764246480
H48	16.6400085293	7.4079289321	3.9087774288
C49	15.1171825111	8.2689762411	5.1616104295
H50	15.7639961060	8.3450622173	6.0320772034
C51	13.7940312522	8.7240089313	5.2479699145
H52	13.4185376760	9.1619677473	6.1676305397
C53	12.9616736218	8.6153314456	4.1332181175
C54	11.0265003502	9.7363284877	5.0732259610
H55	10.9984482698	9.1257460727	5.9864643029
H56	9.9994435036	9.9531416815	4.7780183601
H57	11.5489728314	10.6797893631	5.2973039476
N58	9.5701711624	8.3662132449	2.8328977818
N59	10.7605668875	9.0424380829	0.5705739548
N60	12.4656763995	8.0794872865	1.9516591984
N61	11.6711477010	9.0163155837	4.0067688982
P62	10.9732456320	8.9544166989	2.3678076581
F63	10.9962679819	10.6178776246	2.3525038285

$Ph_3P{=}NPh$

E(M06-2X/6-311+G**) = -1322.511101829

H(M06-2X/6-31+G*) = -1321.864826

E(BP86/6-31G*) = -1322.684667119

C1	0.0373849229	5.4267982798	6.2100639824
C2	-1.0165348485	4.9163336101	6.9678202958
C3	-1.2489552530	3.5438263242	7.0006906904
C4	-0.4269657764	2.6787404292	6.2716031837
C5	0.6323704744	3.1887344294	5.5185432181
C6	0.8613142584	4.5633807122	5.4901870521
H7	0.2191040700	6.4973886205	6.1868179026
H8	-1.6531575530	5.5859659024	7.5383312907
H9	-2.0575167754	3.1497188222	7.6119740872
H10	1.2694574847	2.4951247809	4.9778089062
H11	1.6870985290	4.9599709527	4.9070405656
C12	-4.4223998669	0.3027454324	3.5258690785
C13	-3.1722286268	-0.1898907093	3.1591831845
C14	-2.0769012905	-0.0174399365	4.0048412279
C15	-2.2350196619	0.6432203873	5.2257022944
C16	-3.4933235763	1.1367453147	5.5909534860
C17	-4.5833452772	0.9684434827	4.7419661322
H18	-5.2737298406	0.1701537526	2.8645919418
H19	-3.0462959914	-0.7084520723	2.2135882539
H20	-1.0961498103	-0.3929428065	3.7237438897
H21	-3.6283226966	1.6497804364	6.5399341129
H22	-5.5570216634	1.3551776665	5.0277957206
C23	-1.7689519974	-0.2464694689	10.5998849664
C24	-0.6894808373	0.5888270777	10.3111233470
C25	-0.4179760038	0.9433520991	8.9933092761
C26	-1.2292247636	0.4705782289	7.9541425420
C27	-2.3022811755	-0.3753342453	8.2482676892
C28	-2.5716347236	-0.7300798150	9.5693350223
H29	-1.9809783194	-0.5237056433	11.6283163952

H30	-0.0583362709	0.9615121545	11.1121406688
H31	0.4277721877	1.5889250066	8.7670788725
H32	-2.9316366705	-0.7597121524	7.4494597156
H33	-3.4073301650	-1.3870463737	9.7911633742
P34	-0.7343627740	0.8904718409	6.2441011953
N35	0.5788004878	0.2217950264	5.6734469149
C36	1.5487304477	-3.8627075944	5.2264199944
C37	2.4581161673	-2.8471741303	4.9203233802
C38	2.1130825910	-1.5123989019	5.0824936366
C39	0.8397921908	-1.1372968021	5.5564480367
C40	-0.0669411560	-2.1726590215	5.8601953098
C41	0.2868400574	-3.5106223028	5.6974434137
H42	1.8205384240	-4.9060148623	5.0998918589
H43	3.4491681082	-3.0996312380	4.5521258200
H44	2.8193537964	-0.7209547152	4.8484661872
H45	-1.0621124348	-1.9299797154	6.2255624494
H46	-0.4376542858	-4.2831804002	5.9421167803

$Ph_3P{=}NPh\text{-}H^+$

E(M06-2X/6-311+G**) = -1322.926215820

H(M06-2X/6-31+G*) = -1322.26305

C1	-0.0472572328	5.4962446212	6.3076604130
C2	-0.0384192416	4.7622287719	7.4925986020
C3	-0.2985255165	3.3945193901	7.4690256714
C4	-0.5703473238	2.7702274555	6.2462598439
C5	-0.5930109115	3.5084196275	5.0539411614

C6	-0.3239642900	4.8724739568	5.0904154662
H7	0.1541287319	6.5625885120	6.3328025594
H8	0.1659626665	5.2545153661	8.4376848546
H9	-0.3017841260	2.8256385884	8.3944079679
H10	-0.8314983190	3.0254029212	4.1090188631
H11	-0.3391191310	5.4498342562	4.1718486440
C12	-4.2924726880	0.2929685766	3.2251970401
C13	-3.1000275280	-0.4114976121	3.0743779419
C14	-2.0493642078	-0.2063415205	3.9662548504
C15	-2.2077358653	0.7081470284	5.0125493575
C16	-3.3999887461	1.4327209698	5.1554330494
C17	-4.4424216458	1.2169637541	4.2611307750
H18	-5.1068360290	0.1313177389	2.5259563020
H19	-2.9824347735	-1.1172215711	2.2585939622
H20	-1.1133058100	-0.7435784065	3.8396791890
H21	-3.5073946842	2.1731310058	5.9456894226
H22	-5.3666411188	1.7761283712	4.3643531769
C23	-1.6713378529	-0.7119784623	10.3225089115
C24	-0.3684866319	-0.4033859599	9.9282023377
C25	-0.1301681319	0.1056618512	8.6566535001
C26	-1.2073653965	0.3090346480	7.7825106582
C27	-2.5123083924	-0.0110722279	8.1704030372
C28	-2.7384940976	-0.5197570330	9.4471779607
H29	-1.8532889359	-1.1139964517	11.3142352177
H30	0.4616695086	-0.5691962909	10.6068980888
H31	0.8864295916	0.3239396323	8.3376162840
H32	-3.3444445213	0.1173430981	7.4842344083
H33	-3.7480532981	-0.7728001113	9.7539534517
P34	-0.8589710757	0.9994448421	6.1625795040
C35	1.9368777869	-3.6374292648	5.8835733477

C36	2.8204011718	-2.5896675497	5.6298105214
C37	2.3560974472	-1.2813285621	5.5469745905
C38	0.9937423850	-1.0167644531	5.7045389793
C39	0.1005636900	-2.0611125142	5.9508715820
C40	0.5813712586	-3.3658845144	6.0455903664
H41	2.3024310181	-4.6563708193	5.9521701714
H42	3.8797333185	-2.7867327986	5.5001908842
H43	3.0507479531	-0.4658172005	5.3601558010
H44	-0.9636681508	-1.8749995141	6.0704739897
H45	-0.1172028596	-4.1732944705	6.2405725530
N46	0.5608277470	0.3371160666	5.6060010943
H47	1.2498265700	0.9979695106	5.2597882140

Ph_3P=NPh-Me^+

E(M06-2X/6-311+G**) = -1362.216090551

H(M06-2X/6-31+G*) = -1361.514391

C1	-0.3261552774	5.5311804115	6.2968065282
C2	-0.4878660458	4.8707539700	7.5119135892
C3	-0.6001053285	3.4811343041	7.5436423333
C4	-0.5479114065	2.7621914952	6.3459974737
C5	-0.3987190781	3.4266109367	5.1196492008
C6	-0.2830834886	4.8108173854	5.1005144965
H7	-0.2405805503	6.6131774447	6.2775078447
H8	-0.5318385661	5.4345647838	8.4380080597
H9	-0.7346798681	2.9696725290	8.4922707330
H10	-0.3816800361	2.8654077909	4.1877090124
H11	-0.1673386341	5.3302536960	4.1547838568

C12	-3.8777539185	0.0684119625	3.1709245523
C13	-2.6801003304	-0.6406275601	3.1273598909
C14	-1.6857581210	-0.4061562818	4.0755709171
C15	-1.9005562040	0.5530539631	5.0718920023
C16	-3.0998993718	1.2830969156	5.1030921313
C17	-4.0873542871	1.0327288868	4.1573576990
H18	-4.6470636358	-0.1220760967	2.4292060863
H19	-2.5127054524	-1.3811643405	2.3520894697
H20	-0.7586429655	-0.9661594609	4.0254081769
H21	-3.2556757454	2.0593121471	5.8495734388
H22	-5.0130783092	1.5983847333	4.1825035423
C23	-1.9006607086	-0.3578217518	10.5356792086
C24	-0.5710458254	-0.0459656870	10.2459646479
C25	-0.2136755823	0.3355097530	8.9573758686
C26	-1.1952113414	0.4114140316	7.9593805648
C27	-2.5252305936	0.0895187135	8.2448321506
C28	-2.8723831081	-0.2946799199	9.5388445524
H29	-2.1770983008	-0.6614886628	11.5405080979
H30	0.1865813300	-0.1099256745	11.0202362119
H31	0.8258815093	0.5531033300	8.7213478413
H32	-3.2834963320	0.1173632576	7.4678760611
H33	-3.9022140378	-0.5517962838	9.7646116227
P34	-0.6714616462	0.9670048643	6.3261410471
C35	1.4252737583	-3.7138400205	4.9874254890
C36	2.1587352541	-2.7136786434	4.3533977131
C37	1.9669950911	-1.3756738502	4.6880502722
C38	1.0431557566	-1.0269631269	5.6791878566
C39	0.3194024177	-2.0304915080	6.3314802502
C40	0.5065134067	-3.3638778866	5.9732961887
H41	1.5735034386	-4.7548255137	4.7204168556

H42	2.8808295280	-2.9695024190	3.5843911599
H43	2.5279948799	-0.6085056999	4.1649008945
H44	-0.3859428693	-1.7904537011	7.1191563332
H45	-0.0641780978	-4.1326531296	6.4845952399
N46	0.8461310244	0.3622818138	5.9884047449
C47	2.0080636750	1.2558529884	5.8312047846
H48	2.8963190997	0.7023503004	6.1415591026
H49	2.1330481538	1.5932561557	4.7971240104
H50	1.9043547760	2.1298804471	6.4731493698

$Ph_3P{=}NPh\text{-}F^-$

E(M06-2X/6-311+G**) = -1422.416484147

H(M06-2X/6-31+G*) = -1421.737960

C1	0.5642866921	4.9460731679	5.5218752245
C2	0.3222641051	4.4894127275	6.8163910203
C3	-0.1321974112	3.1872876103	7.0282574234
C4	-0.3764278916	2.3364413300	5.9489107698
C5	-0.1409013730	2.8032524700	4.6535132105
C6	0.3382643662	4.0940996721	4.4405775483
H7	0.9275270330	5.9573630840	5.3567650756
H8	0.4977043867	5.1447935638	7.6664790674
H9	-0.2958983490	2.8349712305	8.0429322668
H10	-0.3369781963	2.1388134768	3.8141907796
H11	0.5280930842	4.4394087023	3.4271379987
C12	-5.1591108466	2.0881627119	4.2958902973
C13	-4.4540453934	1.0637617288	3.6679564362
C14	-3.2383145150	0.6153771078	4.1942002274
C15	-2.6991620384	1.1765342981	5.3557188819

C16	-3.4210994186	2.2114253613	5.9681954735
C17	-4.6345252523	2.6637433098	5.4549834856
H18	-6.1050003056	2.4379696296	3.8885805949
H19	-4.8512488259	0.6077722940	2.7631494609
H20	-2.6791034697	-0.1843364519	3.7169291492
H21	-3.0291365577	2.6744942328	6.8742534104
H22	-5.1716618906	3.4659250897	5.9566690266
C23	-3.0781114536	-0.6165092155	10.1556710758
C24	-1.8401067370	0.0220936412	10.1836326897
C25	-1.2124569369	0.3934821051	8.9937547130
C26	-1.8293338347	0.1752904151	7.7550870753
C27	-3.0707901618	-0.4732303290	7.7433581865
C28	-3.6842821647	-0.8778670317	8.9274912801
H29	-3.5616100376	-0.9183815733	11.0815881621
H30	-1.3480749168	0.2157455502	11.1338689646
H31	-0.2199616978	0.8286322949	9.0193169001
H32	-3.5601704597	-0.6702470526	6.7933232662
H33	-4.6409030076	-1.3927252541	8.8891658669
N34	-0.7381349778	-0.4697173315	4.9458354556
C35	1.8216381334	-3.8243284972	4.7521368257
C36	1.5253448514	-3.0528089166	3.6264885653
C37	0.7053759785	-1.9342945446	3.7248643127
C38	0.1371914451	-1.5261622617	4.9557060337
C39	0.4476835162	-2.3255545441	6.0840235456
C40	1.2685774131	-3.4418499197	5.9774245730
H41	2.4625703898	-4.6989887721	4.6779460517
H42	1.9405624115	-3.3246827586	2.6572372038
H43	0.4741720523	-1.3377839635	2.8454599144
H44	0.0342133030	-2.0476400963	7.0489094659
H45	1.4809781691	-4.0267662835	6.8709593653

P46	-1.0166684807	0.5990714803	6.1178576137
F47	0.5146351922	0.3350174866	6.9757411138

Ph_3P=NPh-He_8-ring complex at 1.7 Å

E(BP86/6-31G*) = -1345.80204608

He1	2.0198000000	1.8633000000	11.4447000000
He2	6.2280000042	3.2546000085	9.1306999790
He3	4.8860000000	0.1785000000	10.2418000000
He4	3.3618000000	4.9395000000	10.3336000000
He5	3.1955000000	0.3896000000	11.1134000000
He6	5.0726000055	4.7343999865	9.5021000131
He7	6.1504000089	1.3674000025	9.4372000176
He8	2.0974000000	3.7505000000	11.1382000000
X9	4.1239000000	2.5590000000	10.2877000000
P10	3.7918598338	2.3082223504	7.2020076611
N11	3.3670999814	2.3457000025	8.7830999903
C12	-0.8866148136	1.8119380854	9.1341134939
C13	-0.0208655247	0.7067369890	9.0952820345
C14	1.3629576327	0.8903234266	8.9739588262
C15	1.9357257806	2.1827993412	8.8902877435
C16	1.0450111472	3.2833502753	8.9179262677
C17	-0.3410469115	3.1020557128	9.0422189322
H18	-1.9690221499	1.6695817390	9.2296130326
H19	-0.4264680761	-0.3108210441	9.1552333919
H20	2.0323867325	0.0238332481	8.9382359231
H21	1.4547374115	4.2963839635	8.8458504508

H22	-0.9991617117	3.9798560175	9.0624980394
C23	0.7598935734	0.2363144173	4.2724285259
C24	1.9809148265	-0.3955802618	4.5470308154
C25	2.9116379196	0.2022834317	5.4131353076
C26	2.6374601752	1.4472990907	6.0153415026
C27	1.4084536839	2.0824533103	5.7180643370
C28	0.4786269865	1.4800029365	4.8608441146
H29	0.0342070154	-0.2327417748	3.5983967259
H30	2.2193831002	-1.3597570452	4.0831871561
H31	3.8663344259	-0.2999797447	5.5936471541
H32	1.1735298987	3.0526292028	6.1657178643
H33	-0.4703911722	1.9867557661	4.6525743762
C34	7.8314338744	0.1100294770	6.4418713499
C35	7.7206903008	1.4679574715	6.1106837999
C36	6.5187927589	2.1562511335	6.3404904321
C37	5.4162213449	1.4924933773	6.9127809903
C38	5.5459707127	0.1312876577	7.2680914942
C39	6.7413778269	-0.5578062330	7.0239163912
H40	8.7683349038	-0.4269936229	6.2550017761
H41	8.5734101399	1.9982547776	5.6717539642
H42	6.4429314414	3.2153067103	6.0764411997
H43	4.7129051385	-0.3799941809	7.7624753464
H44	6.8265404701	-1.6148939674	7.3000728506
C45	4.0153048697	6.4532757338	5.0351853426
C46	3.7473872766	6.3852886059	6.4095754077
C47	3.7028427974	5.1395675460	7.0574558630
C48	3.9221970305	3.9526145792	6.3377961401
C49	4.1747946046	4.0278315939	4.9490079858
C50	4.2283878227	5.2711948352	4.3046103326
H51	4.0506343701	7.4246127678	4.5285844049

H52	3.5715309462	7.3029447529	6.9825576414
H53	3.4935015362	5.0769190975	8.1272377407
H54	4.3197391880	3.1091738860	4.3688417029
H55	4.4283533404	5.3183656066	3.2278636616

Ph_3P=NPh-He_8-ring complex at 2.2 Å

E(BP86/6-31G*) = -1345.816179790

He1	2.0198000000	1.8633000000	11.4447000000
He2	6.2280000149	3.2546000333	9.1306999137
He3	4.8860000000	0.1785000000	10.2418000000
He4	3.3618000000	4.9395000000	10.3336000000
He5	3.1955000000	0.3896000000	11.1134000000
He6	5.0725999871	4.7343999006	9.5021000332
He7	6.1504000408	1.3674000115	9.4372000811
He8	2.0974000000	3.7505000000	11.1382000000
X9	4.1239000000	2.5590000000	10.2877000000
P10	3.6325620921	2.5657530081	6.8215871739
N11	3.1430999572	2.2826000546	8.3378999720
C12	-1.0576296417	1.8901180070	9.0612241937
C13	-0.1599597879	0.8465755293	9.3417487145
C14	1.2084782521	0.9960617533	9.0880436856
C15	1.7385813370	2.1979429638	8.5532468265
C16	0.8144715863	3.2359054382	8.2697820403
C17	-0.5571620116	3.0832373236	8.5197804305
H18	-2.1295338483	1.7722792091	9.2565170925
H19	-0.5300860131	-0.0997694707	9.7558753231
H20	1.9042944786	0.1784597681	9.3004835819

H21	1.1761274555	4.1744240013	7.8358638438
H22	-1.2401884559	3.9085863383	8.2828579527
C23	0.7068111721	0.7776895285	3.6365022604
C24	1.0314539109	0.0753846074	4.8075316193
C25	1.9042453478	0.6392060128	5.7476062806
C26	2.4761616759	1.9130905251	5.5251392670
C27	2.1245275242	2.6195604336	4.3572715158
C28	1.2495330093	2.0520824143	3.4178440801
H29	0.0216184463	0.3376088299	2.9030242688
H30	0.5935610814	-0.9107945922	4.9983804366
H31	2.1158605678	0.1035551415	6.6781517869
H32	2.5226627770	3.6229905346	4.1798302322
H33	0.9870066294	2.6149150228	2.5146735416
C34	7.6882081143	0.4103720990	5.9762325708
C35	7.6754721205	1.7932204265	6.2080582628
C36	6.4640055082	2.4567078007	6.4567703833
C37	5.2489550385	1.7421872122	6.4812836675
C38	5.2736267356	0.3501629053	6.2502461796
C39	6.4831510176	-0.3101902442	5.9983428161
H40	8.6342822614	-0.1059316153	5.7774785359
H41	8.6119627056	2.3624729308	6.1972875552
H42	6.4688746538	3.5357980403	6.6346873398
H43	4.3412216077	-0.2224112271	6.2568704279
H44	6.4833924593	-1.3906662923	5.8155275481
C45	4.3279476583	7.0357907050	5.6218001572
C46	3.7062507120	6.7024624765	6.8339681534
C47	3.5190164624	5.3552797296	7.1816118084
C48	3.9461004010	4.3267913066	6.3213122405
C49	4.5837227271	4.6716774458	5.1070606392
C50	4.7700789366	6.0180327819	4.7599169382

H51	4.4756883010	8.0870924151	5.3496097782
H52	3.3698740115	7.4912960807	7.5162231612
H53	3.0550924524	5.0908428520	8.1355219753
H54	4.9447688950	3.8856961904	4.4337346212
H55	5.2652077775	6.2727606679	3.8157542057

7. References

[1] J. Kobayashi, T. Agou, T. Kawashima. *Chem. Lett*. **2003**, *32*, 1144−1145.

[2] T. Shioiri, *TCI MAIL.* **2007**, *134*, 2.

[3] Rigaku Oxford Diffraction, **2020**, CrysAlisPro Software system, version 1.171.40.82a, Rigaku Corporation, Wroclaw, Poland.

[4] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, *42*, 339–341.

[5] [a)] C. B. Hübschle, G. M.; Sheldrick, B. Dittrich, *J. Appl. Crystallogr.* **2011**, *44*, 1281–1284. [b)] G. M. Sheldrick, *Acta Crystallogr. Sect. A Found. Crystallogr.* **2015**, *71*, 3–8.

[6] Jaguar 8.5, Schrodinger, Inc., New York, NY, **2014**.

[7] K. O. Christe, D. A. Dixon, D. McLemore, W. W. Wilson, J. A. Sheehy, J. A. Boatz, *J. Fluorine Chem*., **2000**, *101*, 151–153.

[8] J. W. Larson, T. B. McMahon, *Inorg. Chem*. **1987**, *26*, 4018, and references cited therein.

[9] P. Erdmann, J. Leitner, J. Schwarz, L. Greb, Chem. Phys. Chem. 2020, 21, 987-994.

[10] NBO 6.0. E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, and F. Weinhold (Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, 2013)

[11] J. Jover, N. Fey, M. Purdie, G. C. Lloyd-Jones, J. N. Harvey, *J. Mol. Catal. A. Chem*., **2010**, *324*, 39–47.

[12] Falivene, L., Cao, Z., Petta, A. *et al.* Towards the online computer-aided design of catalytic pockets. *Nat. Chem.* **11**, 872–879 (2019).

[13] F. M. Bickelhaupt, K. N. Houk, *Angew. Chem. Int. Ed.,* **2017**, 56, 10070–10086.