Supporting Information

Direct Arylations for Study of the Air-Stable P-Heterocyclic Biradical: From Wide Electronic Tuning to Characterization of the Localized Radicalic Electrons

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Contents

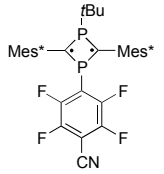
Preparation of Compounds 3–5

General

All manipulations were carried out under an argon atmosphere by the standard Schlenk technique. All solvents employed were dried by appropriate methods. ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded with a Bruker AV300M spectrometer with Me_4Si (^{1}H, ^{13}C) and H_3PO_4 (^{31}P) as internal and external standards. Mass spectra were recorded with a JEOL JMS-T100CS and JMS-700 spectrometers. UV-Vis spectra were recorded with a JASCO V-570 spectrometer. Electrochemical analyses were performed with an ALS 620Ds voltammetric analyzer. Compound **1**[S1] and **B**[S2] was prepared according to the previous papers.

3: To a solution of **1** (500 mg, 1.73 mmol) in THF (10 mL) was added *t*-butyllithium (0.87 mmol, 1.6 M solution in pentane) slowly at –78 °C and stirred for 15 min. The reaction mixture was allowed to warm to room temperature. To the reaction mixture including **2** was added pentafluoropyridine (282 μL, 2.60 mmol) and the mixture was stirred for 36 h at room temperature. The volatile materials were removed *in vacuo*, and the residual solid was dissolved in dichloromethane and filtered off. The solution was concentrated *in vacuo*, and residual solid was washed with hexane and methanol to afford **3** as an air-stable blue solid (295 mg, 43% yield). Mp 176–179 °C (decomp.); ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.91 (d, ^{3}J(P,H) = 15.9 Hz, 9H, *t*BuP), 1.30 (s, 18H, *p*-*t*Bu), 1.49 (s, 18H, *o*-*t*Bu), 1.61 (s, 18H, *o*-*t*Bu), 7.33 (s, 2H, *m*-Mes*), 7.46 (s, 2H, *m*-Mes*); $^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$) δ –22.8 (dt, ^{2}J(P,P) = 221.4 Hz, ^{3}J(P,F) = 29.2 Hz PPy), 87.0 (d, ^{2}J(P,P) = 221.4 Hz *t*BuP); ^{19}F NMR (282 MHz, $CDCl_3$) δ –124.3, –123.9 (m, 3-py), –93.2, –92.9 (m, 2-Py); UV/Vis (CH_2Cl_2) λ_{max} (ε): 351 (17,000), 608 (1,100) nm; ESI-MS Calcd. for $C_{47}H_{68}F_4NP_2$: 784.4763, Found: 784.4799. ^{13}C NMR spectrum could not be obtained due to the low solubility in any solvent.

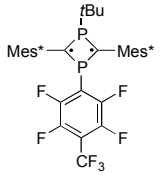
[Cf. 1] Reaction of **2** with pentafluorobenzonitrile gave the mixture containing 1-*t*-butyl-3-(4-cyano-2,3,5,6-tetrafluorophenyl)-2,4-bis(2,4,6-tri-*t*-butylphenyl)-1,3-diphosph acyclobutane-2,4-diyl.



$^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$) δ –21.3 (dt, ^{2}J(P,P) = 223.0 Hz, ^{3}J(P,F) = 34.5 Hz PAryl),

86.8 (d, ^{2}J(P,P) = 223.0 Hz *t*BuP). ^{19}F NMR signals could not be assigned.

[Cf. 2] Reaction of **2** with octafluorotoluene gave the mixture containing 1-*t*-butyl-3-(4-trifluoromethyl-2,3,5,6-tetrafluorophenyl)-2,4-bis(2,4,6-tri-*t*-butylphenyl)-1,3-diphosphacyclobutane-2,4-diyl.



^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ –23.5 (dt, ^{2}J(P,P) = 234.0 Hz, ^{3}J(P,F) = 35.4 Hz PAryl), 84.7 (d, ^{2}J(P,P) = 234.0 Hz *t*BuP); ^{19}F NMR (282 MHz, $CDCl_3$) δ –56.2 (t, ^{4}J(F,F) =21.1 Hz), –119.5 (m), –141.1 (m).

4: To a solution of **3** (20 mg, 25.5 μmol) in THF (10 mL) was added phenyllithium (0.13 mmol, 1.0 M solution in cyclohexane-diethylether) slowly at 0 °C. The reaction mixture was allowed to warm to room temperature and was stirred for 6 h. The volatile materials were removed *in vacuo*, and the residual solid was dissolved in dichloromethane and filtered off. The solution was concentrated *in vacuo*, and the residual solid was washed with methanol to afford **4** as a blue solid (16 mg, 71% yield). Mp 149–152 °C (decomp.); ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.94 (d, ^{3}J(P,H) = 15.3 Hz, 9H, *t*BuP), 1.33 (s, 18H, *p*-*t*Bu), 1.54 (s, 18H, *o*-*t*Bu), 1.65 (s, 18H, *o*-*t*Bu), 7.35–7.38 (m, 8H), 7.48 (s, 2H, *m*-Mes*), 7.80–7.83 (m, 4H); ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ –21.8 (dt, ^{2}J(P,P) = 247.9 Hz, ^{3}J(P,F) = 24.9 Hz, PPy), 79.2 (d, ^{2}J(P,P) = 247.9 Hz *t*BuP); ^{19}F NMR (282 MHz, $CDCl_3$) δ –104.9 (d, ^{3}J(P,F) = 25.7 Hz); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 29.4 (pt, {^{2}J(P,C)+^{4}J(P,C)}/2 = 3.8 Hz, PC*Me*$_3$), 31.6 (s, *p*-C*Me*$_3$), 33.6 (d, ^{5}J(P,C) = 10.6 Hz, *o*-C*Me*$_3$), 34.8 (s, *p*-*C*Me$_3$), 35.0 (s, *o*-C*Me*$_3$), 38.3 (s, *o*-*C*Me$_3$), 39.3 (s, *o*-*C*Me$_3$), 49.3 (dd, ^{1}J(P,C) = 40.4 Hz, ^{3}J(P,C) = 2.6 Hz, P*C*Me$_3$), 97.8 (dd, ^{1}J(P,C) = 29.1 Hz, ^{1}J(P,C) = 21.5 Hz, CP_2), 121.4 (s, *m*-Mes*), 123.5 (d, ^{4}J(P,C) = 2.3 Hz, *m*-Mes*), 128.4 (s, *o*-Ph), 128.9 (s, *p*-Ph), 128.9 (s, *m*-Ph), 131.7 (d, ^{2}J(P,C) = 5.3 Hz, *ipso*-Mes*), 135.5 (dd, ^{3}J(F,C) = 12.8 Hz, ^{5}J(F,C) = 5.3 Hz, *ipso*-Ph), 141.3 (dd, 2-Py) 146.2 (dd, *p*-Mes*), 148.5 (d, ^{3}J(P,C) = 10.6 Hz, *o*-Mes*), 151.3 (dd, ^{3}J(P,C) = 8.7 Hz, ^{3}J(P,C) = 6.4 Hz, *o*-Mes*), 153.9 (ddd, ^{1}J(F,C) = 265.0 Hz, ^{3}J(F,C) = 9.1 Hz, J(P,C) = 4.5 Hz, 3-Py) (4-Py was not determined); UV/Vis (CH_2Cl_2) λ_{max} (ε): 351 (21,000), 596 (1,200) nm; ESI-MS Calcd. for $C_{59}H_{78}F_2NP_2$: 900.5578, Found: 900.5591.

5a: To a solution of **1** (1.00 g, 3.47 mmol) in THF (40 mL) was added *t*-butyllithium (1.73 mmol) slowly at –78 °C and stirred for 15 min. The reaction mixture was allowed to warm to room temperature. To the reaction mixture was added a solution of 2,4,6-trichloro-1,3,5-triazine (384 mg, 2.08 mmol) in THF (40 mL) and the mixture was stirred for 2 h. The solvent was removed *in vacuo*, and the reaction mixture was dissolved in dichloromethane and filtered off. The solution was concentrated *in vacuo*, and residual solid was washed with hexane and acetonitrile to afford **5a** as a green solid (883 mg, 65% yield). Mp 145–148 °C (decomp.); ^{1}H NMR (300 MHz, CD_2Cl_2) δ 0.81 (d, ^{3}J(P,H) = 15.9 Hz, 9H, *t*BuP), 1.31 (s, 18H, *p*-*t*Bu), 1.49 (s, 18H, *o*-*t*Bu), 1.62 (s, 18H, *o*-*t*Bu), 7.29 (pt, {^{5}J(P,H)+^{5}J(P,H)}/2 = 2.0 Hz, 2H, *m*-Mes*), 7.45 (s, 2H, *m*-Mes*); ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ –16.0 (d, ^{2}J(P,P) = 205.3 Hz, ArP), 86.9 (d, ^{2}J(P,P) = 205.3 Hz *t*BuP); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 29.1 (pt, {^{2}J(P,C)+^{4}J(P,C)}/2 = 3 Hz, PC*Me*$_3$), 31.6 (s, *p*-C*Me*$_3$), 33.5 (d, ^{5}J(P,C) = 8.3 Hz, *o*-C*Me*$_3$), 34.7(s, *p*-*C*Me$_3$), 35.4 (s, *o*-C*Me*$_3$), 37.4 (s, *o*-*C*Me$_3$), 39.0 (s, *o*-*C*Me$_3$), 49.8 (dd, ^{1}J(P,C) = 38.1 Hz, ^{3}J(P,C) = 1.9 Hz, P*C*Me$_3$), 99.2 (dd, ^{1}J(P,C) = 27.2 Hz, ^{1}J(P,C) = 13.6 Hz, CP_2), 120.3 (s, *m*-Mes*), 123.2 (d, ^{4}J(P,C) = 2.3 Hz, *m*-Mes*), 131.4 (d, ^{2}J(P,C) = 5.3 Hz, *ipso*-Mes*), 146.0 (s, *p*-Mes*), 148.4 (d, ^{3}J(P,C) = 10.6 Hz, *o*-Mes*), 151.6 (dd, ^{2}J(P,C) = 10.2 Hz, ^{2}J(P,C) = 7.2 Hz, *o*-Mes*), 169.6 (d, ^{3}J(P,C) = 2.3 Hz, CCl), 187.5 (dd, ^{1}J(P,C) = 68.0 Hz, ^{3}J(P,C) = 38.5 Hz, P*C*N$_2$); UV/Vis (CH_2Cl_2) λ_{max} (ε): 367 (24,000), 692 (1,400) nm; ESI-MS Calcd. for $C_{45}H_{67}Cl_2N_3P_2$: 781.4187, Found: 781.4223.

5b: To a solution of **5a** (60 mg, 76.6 μmol) in THF (6 mL) was added phenyllithium (0.19 mmol) slowly at –78 °C. The reaction mixture was allowed to warm to room temperature and the mixture was stirred for 3 h. The solvent was removed *in vacuo*, and the solid was dissolved in dichloromethane and filtered off. The solution was concentrated *in vacuo*, and residual solid was washed with acetonitrile to afford **5b** as a green solid (20 mg, 31% yield). Mp 157–160 °C (decomp.); ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.82 (d, ^{3}J(P,H) = 15.0 Hz, 9H, *t*BuP), 1.35 (s, 18H, *p*-*t*Bu), 1.46 (s, 18H, *o*-*t*Bu), 1.72 (s, 18H, *o*-*t*Bu), 7.32–7.51 (m, 12H), 8.37–8.40 (m, 4H); ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ –15.9 (d, ^{2}J(P,P) = 250.3 Hz, ArP), 74.3 (d, ^{2}J(P,P) = 250.3 Hz *t*BuP); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 29.2 (pt, {^{2}J(P,C)+^{4}J(P,C)}/2 = 3.8 Hz, PC*Me*$_3$), 31.6 (s, *p*-C*Me*$_3$), 33.4 (d, ^{5}J(P,C) = 9.1 Hz, *o*-C*Me*$_3$), 34.6 (s, *p*-*C*Me$_3$), 35.1 (s, *o*-C*Me*$_3$), 37.5 (s, *o*-*C*Me$_3$), 38.8 (s, *o*-*C*Me$_3$), 48.3 (dd, ^{1}J(P,C) = 43.0 Hz, ^{3}J(P,C) = 5.3 Hz, P*C*Me$_3$), 102.4 (dd, ^{1}J(P,C) = 20.4 Hz, ^{1}J(P,C) = 10.6 Hz, CP_2), 119.9 (s, *m*-Mes*), 122.8 (d, ^{4}J(P,C) = 2.3 Hz, *m*-Mes*), 128.5 (s, arom.), 128.9 (s, arom.), 132.3 (s, arom.), 132.7 (d, ^{2}J(P,C) = 3.8 Hz, *ipso*-Mes*), 135.8 (s, arom.), 145.2 (s, *p*-Mes*), 148.1 (d, ^{3}J(P,C) = 10.6 Hz, *o*-Mes*), 150.8 (dd, ^{3}J(P,C) = 9.8 Hz, ^{3}J(P,C) = 7.6 Hz, *o*-Mes*),

169.0 (d, ^{3}J(P,C) = 3.8 Hz, *C*Ph), 182.6 (dd, ^{1}J(P,C) = 43.8 Hz, ^{3}J(P,C) = 34.7 Hz, P*C*N_2); UV/Vis (CH_2Cl_2) λ_{max} (ε): 369 (21,000), 659 (1,100) nm; APCI-MS Calcd. for $C_{57}H_{78}N_3P_2$: 866.5671, Found: 866.5632.

5c: 5a (100 mg, 0.128 mmol) and sodium *tert*-butoxide (31 mg, 0.323 mmol) were dissolved in THF (10 mL), and the mixture was stirred for 24 h at room temperature. The solvent was removed *in vacuo*, and the residual solid was dissolved in hexane and filtered off. The hexane solution was concentrated *in vacuo* and residual solid was washed with acetonitrile to afford **5c** as a green solid (78 mg, 71% yield). Mp 137–140 °C (decomp.); ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.82 (d, ^{3}J(P,H) = 15.0 Hz, 9H, *t*BuP), 1.29 (s, 18H, *p*-*t*Bu), 1.34 (s, 18H, *t*BuO), 1.48 (s, 18H, *o*-*t*Bu), 1.66 (s, 18H, *o*-*t*Bu), 7.25 (s, 2H, *m*-Mes*), 7.37 (s, 2H, *m*-Mes*); ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ –13.3 (d, ^{2}J(P,P) = 253.3 Hz, ArP), 72.3 (d, ^{2}J(P,P) = 253.3 Hz *t*BuP); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 28.6 (s, OC*Me*$_3$), 29.4 (pt, {^{2}J(P,C)+^{4}J(P,C)}/2 = 3.8 Hz, PC*Me*$_3$), 31.6 (s, *p*-C*Me*$_3$), 33.9 (d, ^{5}J(P,C) = 8.3 Hz, *o*-C*Me*$_3$), 34.7 (s, *p*-*C*Me$_3$), 35.3 (s, *o*-C*Me*$_3$), 37.7 (s, *o*-*C*Me$_3$), 38.9 (s, *o*-*C*Me$_3$), 48.4 (dd, ^{1}J(P,C) = 43.0 Hz, ^{3}J(P,C) = 5.3 Hz, P*C*Me$_3$), 82.7 (s, O*C*Me$_3$) 101.8 (dd, ^{1}J(P,C) = 20.4 Hz, ^{1}J(P,C) = 10.6 Hz, CP_2), 120.5 (s, *m*-Mes*), 123.2 (d, ^{4}J(P,C) = 2.3 Hz, *m*-Mes*), 132.1 (d, ^{2}J(P,C) = 4.5 Hz, *ipso*-Mes*), 145.4 (s, *p*-Mes*), 148.1 (d, ^{3}J(P,C) = 10.6 Hz, *o*-Mes*), 151.6 (dd, ^{3}J(P,C) = 16.6 Hz, ^{3}J(P,C) = 7.6 Hz, *o*-Mes*), 169.7 (d, ^{3}J(P,C) = 6.8 Hz, *C*O*t*Bu), 184.1 (dd, ^{1}J(P,C) = 80.8 Hz, ^{3}J(P,C) = 34.0 Hz, P*C*N_2); UV/Vis (CH_2Cl_2) λ_{max} (ε): 353 (15,000), 630 (800) nm; APCI-MS Calcd. for $C_{53}H_{85}N_3NaO_2P_2$: 880.6015, Found: 880.5971.

5d: To a solution of **5a** (100 mg, 0.128 mmol) in THF (10 mL) was added diethylamine (0.13mL, 1.28 mmol) at room temperature. After stirring for 9 h at that temperature, the volatile materials were removed *in vacuo*, and the reaction mixture was dissolved in hexane and filtered off. The solvent of hexane solution was removed *in vacuo*, and residual solid was washed with acetonitrile to afford **5d** as a blue solid (96 mg, 88% yield). Mp 137–140 °C (decomp.); ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.76 (d, ^{3}J(P,H) = 14.1 Hz, 9H, *t*BuP), 0.83 (brs, 6H, NCH_2*Me*), 1.09 (brs, 6H, NCH_2*Me*), 1.30 (s, 18H, *p*-*t*Bu), 1.52 (s, 18H, *o*-*t*Bu), 1.67 (s, 18H, *o*-*t*Bu), 3.26 (brs, 4H, NC*H*$_2$Me), 3.41 (brs, 4H, NC*H*$_2$Me), 7.22 (s, 2H, *m*-Mes*), 7.36 (s, 2H, *m*-Mes*); ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ –13.2 (d, ^{2}J(P,P) = 290.4 Hz, ArP), 63.9 (d, ^{2}J(P,P) = 290.4 Hz *t*BuP); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 13.2 (s, NCH_2*Me*), 29.3 (pt, {^{2}J(P,C)+^{4}J(P,C)}/2 = 3.8 Hz, PC*Me*$_3$), 31.7 (s, *p*-C*Me*$_3$), 33.6 (d, ^{5}J(P,C) = 8.3 Hz, *o*-C*Me*$_3$), 34.7 (s, *p*-*C*Me$_3$), 35.3 (s, *o*-C*Me*$_3$), 37.6 (s, *o*-*C*Me$_3$), 38.9 (s, *o*-*C*Me$_3$), 40.7 (s, N*C*H_2Me), 47.0 (dd, ^{1}J(P,C) = 47.6 Hz, ^{3}J(P,C) = 9.1 Hz, P*C*Me$_3$), 99.2 (dd, ^{1}J(P,C) = 13.6

Hz, ^{1}J(P,C) = 7.6 Hz, CP_2), 119.8 (s, *m*-Mes*), 122.7 (s, *m*-Mes*), 133.9 (d, ^{2}J(P,C) = 4.5 Hz, *ipso*-Mes*), 144.4 (s, *p*-Mes*), 147.9 (d, ^{3}J(P,C) = 10.6 Hz, *o*-Mes*), 150.3 (pt, {^{3}J(P,C)+^{3}J(P,C)}/2 = 8.7 Hz, *o*-Mes*), 162.6 (d, ^{3}J(P,C) = 8.3 Hz, *C*NEt_2), 178.6 (dd, ^{1}J(P,C) = 32.8 Hz, ^{3}J(P,C) = 22.3 Hz, P*C*N_2); UV/Vis (CH_2Cl_2) λ_{max} (ε): 350 (23,000), 627 (1,300) nm; APCI-MS Calcd. for $C_{53}H_{88}N_5P_2$: 856.6515, Found: 856.6479.

5e: To a solution of **5a** (200 mg, 0.255 mmol) in THF (20 mL) was added butylamine (0.25mL, 2.55 mmol) at room temperature. After stirring for 30 min at that temperature, DBU (0.12 mL, 0.769 mmol) was added to the reaction mixture. After stirring for 10 h at that temperature, the volatile materials were removed *in vacuo*, and the reaction products wertr dissolved in hexane and filtered off. The solvent of hexane solution was removed *in vacuo*, and residual solid was washed with acetonitrile to afford **5e** as a blue solid (201 mg, 92% yield). Mp 143–145 °C (decomp.); ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.73 (d, ^{3}J(P,H) = 14.1 Hz, 9H, *t*BuP), 0.83 (brs, 6H, NCH_2*Me*), 1.09 (brs, 6H, NCH_2*Me*), 1.30 (s, 18H, *p*-*t*Bu), 1.53 (s, 18H, *o*-*t*Bu), 1.66 (s, 18H, *o*-*t*Bu), 3.12 (brs, 4H, NC*H_2*Pr), 4.76 (brs, 2H, NH), 7.22 (s, 2H, *m*-Mes*), 7.38 (s, 2H, *m*-Mes*); ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ –14.2 (d, ^{2}J(P,P) = 278.2 Hz, ArP), 68.3 (d, ^{2}J(P,P) = 278.2 Hz *t*BuP); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 13.8 (s, $NCH_2CH_2CH_2$*Me*), 20.0 (s, NCH_2CH_2*C*H_2Me), 29.3 (pt, {^{2}J(P,C)+^{4}J(P,C)}/2 = 3.8 Hz, P*C*Me_3), 31.6 (s, *p*-C*Me_3*), 32.0 (s, NCH_2*C*H_2Et), 33.6 (d, ^{5}J(P,C) = 8.3 Hz, *o*-C*Me_3*), 34.6 (s, *p*-*C*Me_3), 35.5 (s, *o*-C*Me_3*), 37.5 (s, *o*-*C*Me_3), 38.9 (s, *o*-*C*Me_3), 40.3 (s, NH*C*H_2Pr), 47.4 (dd, ^{1}J(P,C) = 46.4 Hz, ^{3}J(P,C) = 7.9 Hz, P*C*Me_3), 104.1 (dd, ^{1}J(P,C) = 16.2 Hz, ^{1}J(P,C) = 7.9 Hz, CP_2), 119.8 (s, *m*-Mes*), 122.9 (s, *m*-Mes*), 133.5 (s, *ipso*-Mes*), 144.6 (s, *p*-Mes*), 147.9 (d, ^{3}J(P,C) = 10.6 Hz, *o*-Mes*), 150.6 (pt, {^{3}J(P,C)+^{3}J(P,C)}/2 = 7.6 Hz, *o*-Mes*), 164.3 (s, ^{3}J(P,C) = 8.3 Hz, CNHBu) (peaks for the P*C*N_2 carbon was not observed). APCI-MS Calcd. for $C_{53}H_{87}N_5P_2$: 855.6437, Found: 855.6397.

5f: To a solution of **5a** (100 mg, 0.128 mmol) and $Pd(PPh_3)_4$ (15 mg, 12.7 μmol) in THF (10 mL) was added dimethylzinc (0.511 mmol, 1.0 M solution in hexane) at room temperature. The reaction mixture was allowed to warm to 30 °C and stirred 24 h. After cooling to room temperature, the volatile materials were removed *in vacuo*, and the reaction products were dissolved in hexane and filtered off. The solvent of hexane solution was removed *in vacuo*, and residual solid was washed with acetonitrile to afford **5f** as a green solid (70 mg, 73% yield). Mp 129–132 °C (decomp.); ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.71 (d, ^{3}J(P,H) = 14.7 Hz, 9H, *t*BuP), 1.30 (s, 18H, *p*-*t*Bu), 1.46 (s, 18H, *o*-*t*Bu), 1.65 (s, 18H, *o*-*t*Bu), 2.40 (s, 6H, Me), 7.24 (s, 2H, *m*-Mes*), 7.38 (s, 2H, *m*-Mes*); ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ –16.3

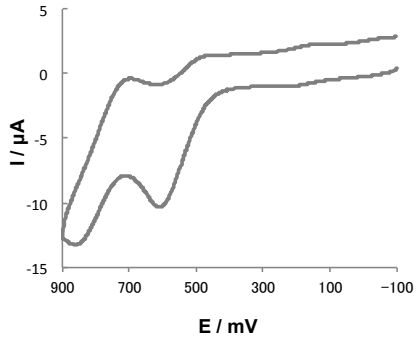
(d, ^{2}J(P,P) = 247.9 Hz, ArP), 77.0 (d, ^{2}J(P,P) = 247.9 Hz *t*BuP); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 25.5 (s, Me), 29.2 (pt, {^{2}J(P,C)+^{4}J(P,C)}/2 = 3.8 Hz, PC*Me*$_3$), 31.6 (s, *p*-C*Me*$_3$), 33.5 (d, ^{5}J(P,C) = 9.1 Hz, *o*-C*Me*$_3$), 34.7 (s, *p*-*C*Me$_3$), 35.5 (s, *o*-C*Me*$_3$), 37.4 (s, *o*-*C*Me$_3$), 38.9 (s, *o*-*C*Me$_3$), 48.4 (dd, ^{1}J(P,C) = 69.3 Hz, ^{3}J(P,C) = 8.5 Hz, P*C*Me$_3$), 99.2 (dd, ^{1}J(P,C) = 20.8 Hz, ^{1}J(P,C) = 10.2 Hz, CP_2), 119.9 (s, *m*-Mes*), 123.0 (d, ^{4}J(P,C) = 2.3 Hz, *m*-Mes*), 132.8 (d, ^{2}J(P,C) = 4.5 Hz, *ipso*-Mes*), 145.2 (s, *p*-Mes*), 148.2 (d, ^{3}J(P,C) = 11.3 Hz, *o*-Mes*), 150.3 (dd, ^{3}J(P,C) = 9.8 Hz, ^{3}J(P,C) = 7.6 Hz *o*-Mes*), 173.9 (d, ^{3}J(P,C) = 3.8 Hz, *C*Me), 181.9 (dd, ^{1}J(P,C) = 44.5 Hz, ^{3}J(P,C) = 34.7 Hz, P*C*N$_2$); UV/Vis (CH_2Cl_2) λ_{max} (ε): 360 (19,000), 643 (1,100) nm; ESI-MS Calcd. for $C_{47}H_{73}N_3NaP_2$: 764.5177, Found: 764.5141.

5g: To a solution of trimetylsilylaccetylene (0.53 mL, 3.83 mmol) in THF (10 mL) was added butyllithium (3.83 mmol, 1.6 M solution in hexane) slowly at –78 °C and stirred for 30 min. The reaction mixture was allowed to warm to 0 °C and added $ZnCl_2$ (3.83 mmol, 1.0 M solution in diethylether). The reaction mixture was allowed to warm to room temperature and stirred for 30 min. To the reaction mixture was added a mixture of **5a** (0.500 g, 0.639 mmol) and $Pd(PPh_3)_4$ (74 mg, 0.0640mmol) in THF (75 mL). The reaction mixture was allowed to warm to 30 °C and stirred for 12 h, and then cooled to room temperature. The volatile materials were removed *in vacuo*, and the reaction mixture was dissolved in hexane and filtered off. The solvent of hexane solution was removed *in vacuo*, and residual solid was washed with acetonitrile to afford **5g** as a blue solid (366 mg, 63% yield). Mp 144–147 °C (decomp.); ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.22 (s, TMS), 0.69 (d, ^{3}J(P,H) = 15.3 Hz, 9H, *t*BuP), 1.30 (s, 18H, *p*-*t*Bu), 1.48 (s, 18H, *o*-*t*Bu), 1.64 (s, 18H, *o*-*t*Bu), 7.25 (s, 2H, *m*-Mes*), 7.41 (s, 2H, *m*-Mes*); ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ –16.4 (d, ^{2}J(P,P) = 232.6 Hz, ArP), 83.0 (d, ^{2}J(P,P) = 232.6 Hz *t*BuP); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ –0.6 (s, TMS), 29.1 (pt, {^{2}J(P,C)+^{4}J(P,C)}/2 = 3.0 Hz, PC*Me*$_3$), 31.6 (s, *p*-C*Me*$_3$), 33.5 (d, ^{5}J(P,C) = 9.1 Hz, *o*-C*Me*$_3$), 34.7 (s, *p*-*C*Me$_3$), 35.6 (s, *o*-C*Me*$_3$), 37.3 (s, *o*-*C*Me$_3$), 39.0 (s, *o*-*C*Me$_3$), 48.9 (dd, ^{1}J(P,C) = 41.5 Hz, ^{3}J(P,C) = 3.8 Hz, P*C*Me$_3$), 100.0 (s, C≡C), 101.0 (s, C≡C), 101.8 (dd, ^{1}J(P,C) = 23.4 Hz, ^{1}J(P,C) = 12.8 Hz, CP_2), 119.9 (s, *m*-Mes*), 123.2 (s, *m*-Mes*), 132.5 (d, ^{2}J(P,C) = 4.5 Hz, *ipso*-Mes*), 145.4 (s, *p*-Mes*), 148.5 (d, ^{3}J(P,C) = 10.6 Hz, *o*-Mes*), 151.4 (dd, ^{2}J(P,C) = 9.8 Hz, ^{2}J(P,C) = 7.6 Hz, *o*-Mes*), 157.3 (d, ^{3}J(P,C) = 3.8 Hz, *C*-C≡C), 183.6 (dd, ^{1}J(P,C) = 55.1 Hz, ^{3}J(P,C) = 36.2 Hz, PCN_2); UV/Vis (CH_2Cl_2) λ_{max} (ε): 368 (27,000), 674 (1,600) nm; ESI-MS Calcd. for $C_{55}H_{85}N_3P_2Si_2$: 905.5757, Found: 905.5799.

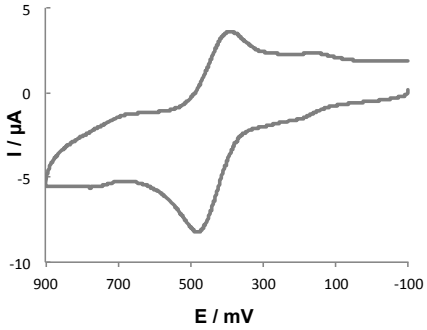
7: To a solution of **1** (200.5 mg, 0.695 mmol) in THF (1.5 ml) was added phenyllithium

(0.723 mmol, 0.64 ml of a 1.13 M solution in butyl ether, 1 M = 1 mol dm^{-3}) at −78 °C and mixture was stirred for 15 min. The mixture was then allowed to warm to temperature, and subsequently mixed with iodine (0.7 mmol). The volatile materials were removed in vacuo, and the residue was extracted with dichloromethane. The hexane extract was concentrated in vacuo, and residual solid was washed with acetonitrile to afford **7** as a deep blue solid (128.7 mg, 51%). Mp 174.0–177.0 °C (decomp.); ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.26 (4H, s, Mes*), 7.00–7.14 (6H, m, Ph), 6.74–6.77 (4H, m, Ph), 1.54 (36H, s, *o*-*t*-Bu), 1.40 (18H, s, *p*-*t*-Bu); ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$) δ = 1.07; ^{13}C{^{1}H} NMR (75.5 MHz, $CDCl_3$) δ = 150.2 (t, $^{3}J_{PC}$ = 6.7 Hz, *o*-Mes*), 146.5 (t, $^{5}J_{PC}$ = 2.3 Hz, *p*-Mes*), 135.6 (pseudo t, ($^{1}J_{PC}$+$^{3}J_{PC}$)/2 = 16.1 Hz, *ipso*-Ph), 132.4 (t, $^{2}J_{PC}$ = 2.3 Hz, *ipso*-Mes*), 128.9 (pseudo t, ($^{2}J_{PC}$+$^{4}J_{PC}$) = 6.8 Hz, *o*-Ph), 128.7 (s, *p*-Ph), 127.9 (s, *m*-Ph), 122.5 (s, *m*-Mes*), 101.2 (t, $^{1}J_{PC}$ = 6.0 Hz, C_{sp2}), 38.2 (s, *o*-*C*Me_3), 35.0 (s, *p*-*C*Me_3), 34.1 (t, $^{5}J_{PC}$ = 4.2 Hz, *o*-C*Me*$_3$), 31.7 (s, *p*-C*Me*$_3$); UV-Vis (CH_2Cl_2) λ_{max} (ε) = 239 (31,000), 367 (33,000), 610 (2,000) nm. APCI-MS Calcd for $C_{50}H_{68}P_2$ 730.4796; found: *m/z* 730.4801.

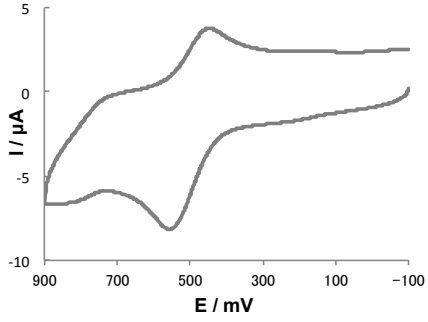
Conditions for cyclic voltammetry: 1 mM in dichloromethane; supporting electrolyte: 0.1 M tetrabutylammonium perchlorate (TBAP); working electrode: glassy carbon; counter electrode: platinum wire; reference electrode: Ag/AgCl ($E_{1/2}$ (ferrocene/ferricinium) = +0.49 V) at 20 °C; scan rate: 50 mV s^{-1}.



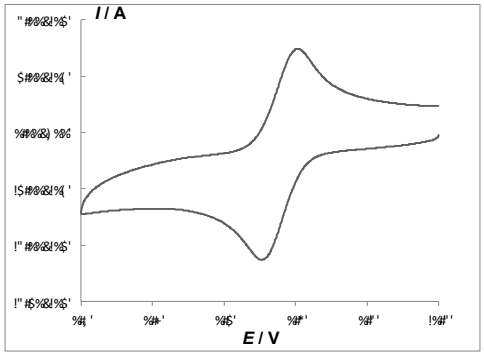
Cyclic Voltammogram of **3**.



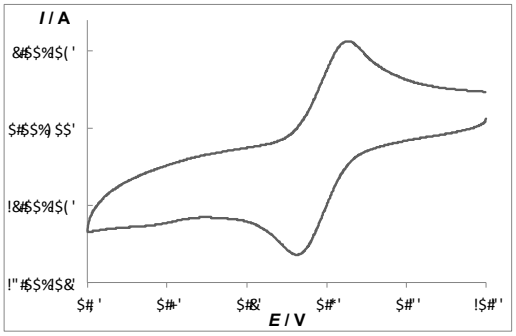
Cyclic Voltammogram of **4**.



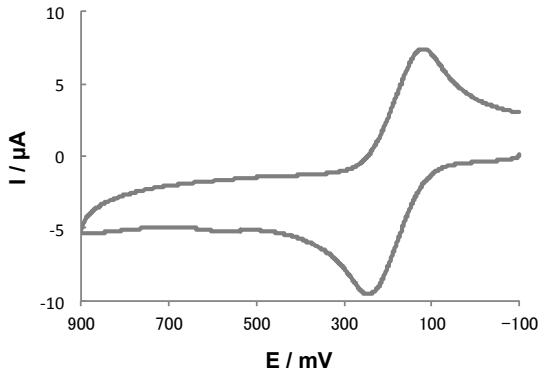
Cyclic Voltammogram of **5a**.



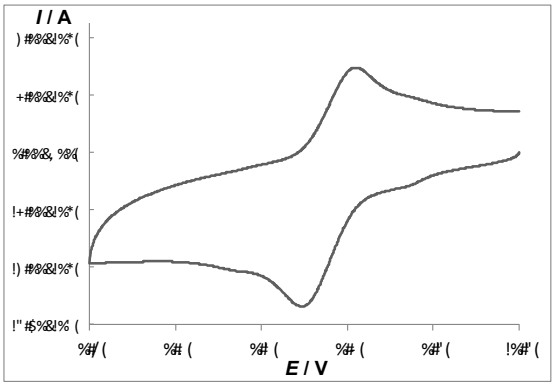
Cyclic Voltammogram of **5b**.



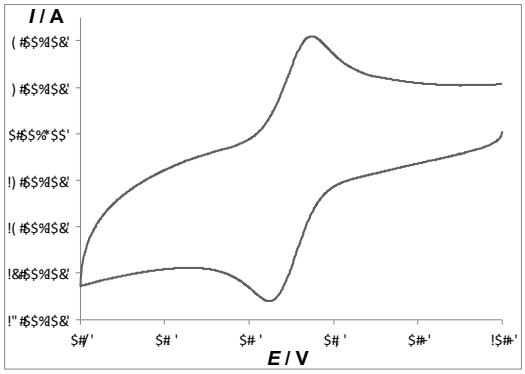
Cyclic Voltammogram of **5c**.



Cyclic Voltammogram of **5d**.



Cyclic Voltammogram of **5f**.



Cyclic Voltammogram of **5g**.

X-ray crystallographic data: 5b: $C_{57}H_{76}N_3P_2 \cdot 0.5CH_2Cl_2$, deep blue prisms (MeOH-CH_2Cl_2), M_W = 908.62, crystal dimensions = 0.39 × 0.32 × 0.19 mm^3, monoclinic, space group *C*2/*c* (#15), a = 26.9518(12), b = 21.0329(8), c = 19.4833(6) Å, β = 101.3701(13)°, V = 10827.8(7) Å^3, Z = 8, λ = 0.71075 Å, T = 123 K, ρ_{calcd} = 1.115 g cm^{-3}, $\mu_{MoK\alpha}$ = 0.167 mm^{-1}, F_{000} = 3928, 46914 total reflections ($2\theta_{max}$ = 54.96°), index ranges = –34≤*h*≤34, –26≤*k*≤27, –25≤*l*≤24, 12368 unique reflections (R_{int} = 0.073), *R*1 = 0.0589 ($I > 2\sigma(I)$), 0.0876 (all data), *wR*2 = 0.1617 ($I > 2\sigma(I)$), 0.1896 (all data), S = 1.170 (903 parameters). **5d**: $C_{53}H_{87}N_5P_2$, deep blue prisms (MeOH-CH_2Cl_2), M_W = 856.22, crystal dimensions = 0.23 × 0.22 × 0.06 mm^3, monoclinic, space group $P2_1/c$ (#14), a = 9.5000(3), b = 26.4002(8), c = 20.6701(5) Å, β = 91.5161(10)°, V = 5182.3(3) Å^3, Z = 4, λ = 0.71075 Å, T = 123 K, ρ_{calcd} = 1.097 g cm^{-3}, $\mu_{MoK\alpha}$ = 0.122 mm^{-1}, F_{000} = 1880, 46451 total reflections ($2\theta_{max}$ = 54.96°), index ranges = –12≤*h*≤12, –34≤*k*≤34, –24≤*l*≤26, 11637 unique reflections (R_{int} = 0.052), *R*1 = 0.0544 ($I > 2\sigma(I)$), 0.0766 (all data), *wR*2 = 0.1507 ($I > 2\sigma(I)$), 0.1721 (all data), S = 1.160 (877 parameters). **5e**: $C_{53}H_{87}N_5P_2$, deep-blue plates (MeOH-CH_2Cl_2), M_W = 856.22, crystal dimensions = 0.26 × 0.15 × 0.08 mm^3, triclinic, space group *P*-1 (#2), a = 9.4039(5), b = 15.7033(8), c = 19.3399(10) Å, α = 70.5365(15),β = 82.3034(17), γ = 88.2449(18)°, V = 2668.2(2) Å^3, Z = 2, λ = 0.71075 Å, T = 123 K, ρ_{calcd} = 1.066 g cm^{-3}, $\mu_{MoK\alpha}$ = 0.119 mm^{-1}, F_{000} = 940, 26573 total reflections ($2\theta_{max}$ = 54.98°), index ranges = –12≤*h*≤12, –20≤*k*≤20, –25≤*l*≤25, 12164 unique reflections (R_{int} = 0.056), *R*1 = 0.0604 ($I > 2\sigma(I)$), 0.1015 (all data), *wR*2 = 0.1544 ($I > 2\sigma(I)$), 0.2293 (all data), S = 1.362 (968 parameters). CCDC-895212 (**5b**), 958909 (**5d**), and 895211 (**5e**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Bond lengths (Å) and angles (°) of X-ray structure of **5b**, **5d**, and **5e**

	5b	**5d**	**5e**
P1–C1	1.720(2)	1.724(2)	1.734(3)
P1–C2	1.712(2)	1.720(2)	1.723(2)
P2–C1	1.780(2)	1.799(2)	1.780(2)
P2–C2	1.780(2)	1.786(2)	1.775(3)
C1–Mes*	1.483(3)	1.484(2)	1.488(3)
C2–Mes*	1.485(3)	1.480(2)	1.475(3)
P1–*t*Bu	1.871(2)	1.867(2)	1.871(3)
P2–C3	1.838(2)	1.847(2)	1.833(3)
C3–N1	1.332(2)	1.329(2)	1.325(3)
N1–C4	1.342(3)	1.360(2)	1.347(3)
C4–N2	1.333(3)	1.339(2)	1.352(3)
N2–C5	1.341(3)	1.338(2)	1.340(3)
C5–N3	1.350(3)	1.362(2)	1.342(3)
C3–N3	1.337(3)	1.334(2)	1.337(3)
C4–Ph/N4	1.470(3)	1.349(2)	1.337(3)
C5–Ph/N5	1.472(4)	1.357(2)	1.355(4)
C1–P1–C2	94.3(1)	93.94(9)	93.9(1)
C1–P1–*t*Bu	124.0(1)	125.64(9)	123.4(1)
C2–P1–*t*Bu	125.1(1)	124.15(9)	121.7(1)
C1–P2–C2	89.96(9)	89.24(8)	90.5(1)
C1–P2–C3	116.25(9)	115.35(8)	114.8(1)
C2–P2–C3	111.31(9)	114.52(8)	116.6(1)
P1–C1–P2	87.60(9)	87.96(8)	87.4(1)
P1–C1–Mes*	124.1(1)	127.7(1)	125.6(2)
P2–C1–Mes*	144.0(2)	142.2(1)	144.7(2)
P1–C2–P2	87.87(9)	88.51(9)	87.9(1)
P1–C2–Mes*	133.7(2)	124.7(1)	127.1(2)
P2–C2–Mes*	138.4(2)	146.5(1)	145.0(2)

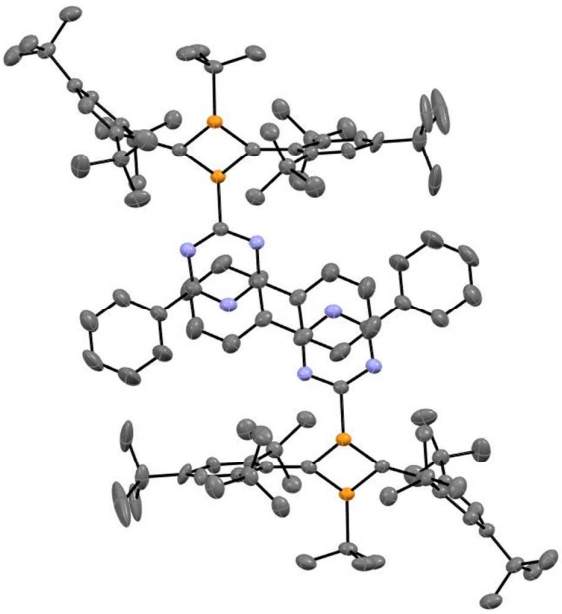


Figure S1. A π-π Stacking mode in the crystal structure of **5b**.

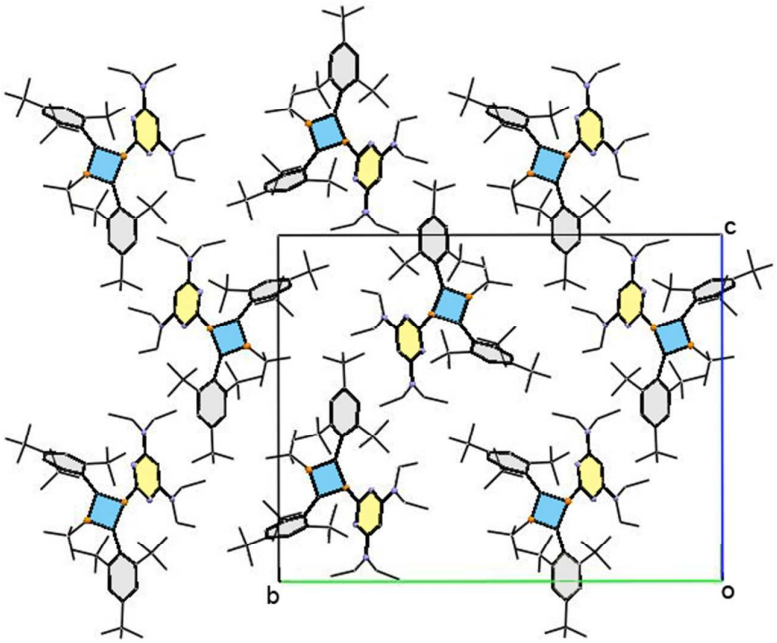


Figure S2. Crystal structure of **5d**.

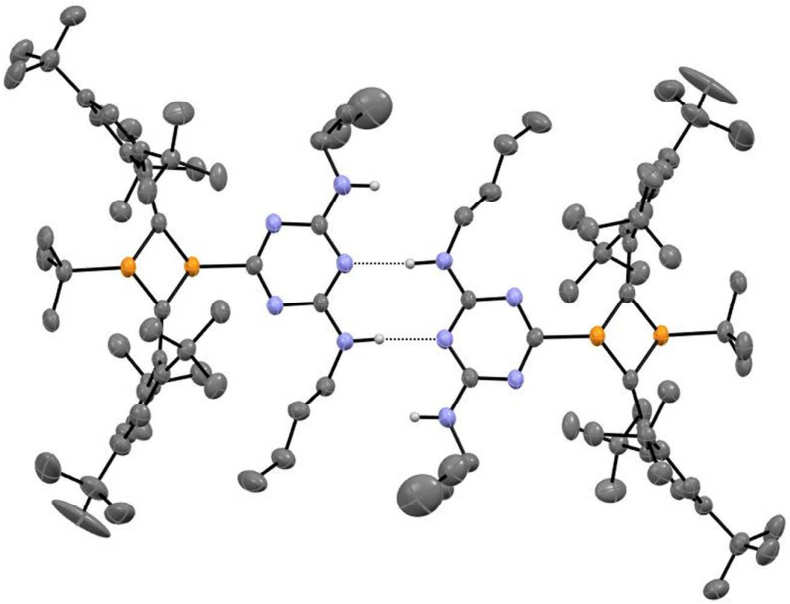


Figure S3. Dimeric structure of **5e** by H-bonds.

Semiconducting Properties

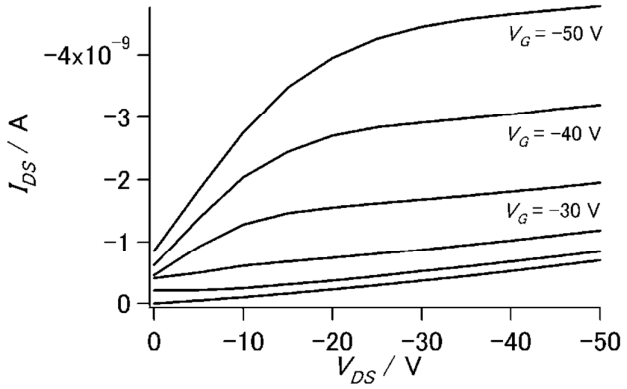


Figure S4. Output curves of an FET based on **5d** by using bare silica dielectric surface.

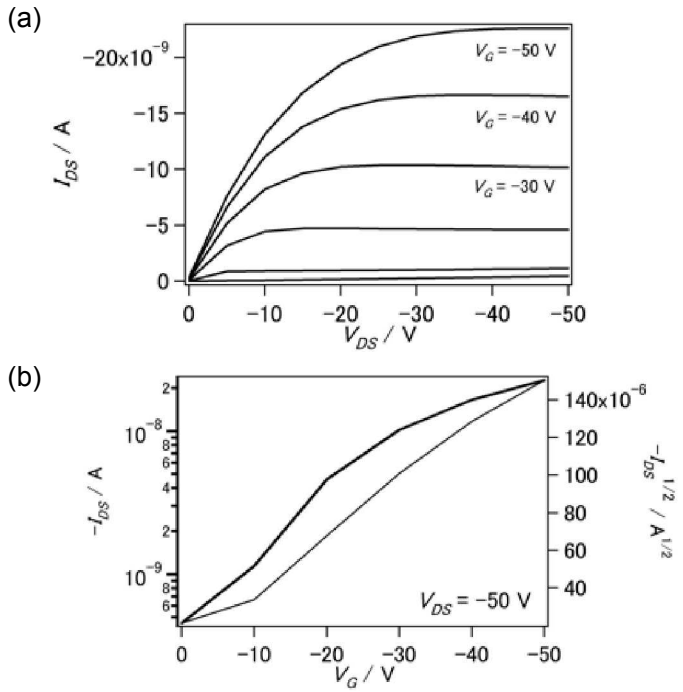


Figure S5. The p-type semiconducting characteristics of an OFET based on **B** by using bare silica dielectric surface. (a) Current-voltage output curves. (b) Transfer plots.
$\mu = 1.67\text{x}10^{-7}$ $cm^2V^{-1}s^{-1}$, on/off ratio = 70, V_{th} = –0.1 V.

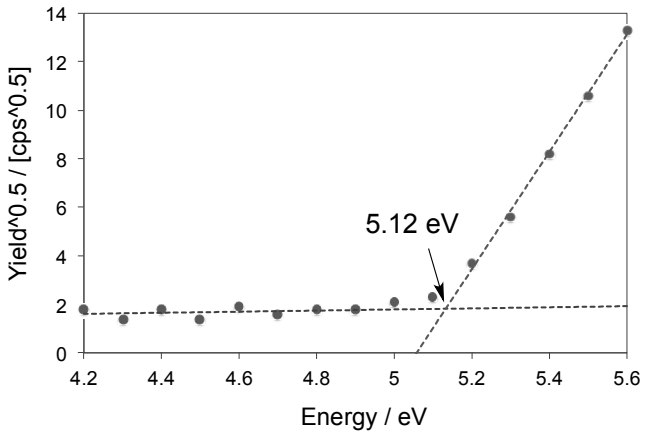
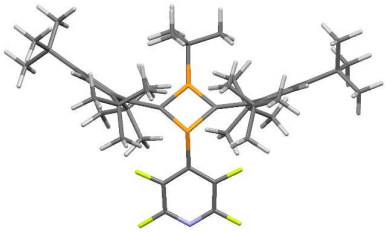


Figure S6. Photoelectron yield spectroscopy in air of crystalline **B**.

DFT Calculation Data of **3–5**

DFT calculations were carried out with Gaussian 09 program package.[S3] The structures were optimize by use of the M06-2X Hamiltonian accounting for the "medium-range" correlations[S4,S5] and the 6-31G(d) basis sets.

3



opt m062x/6-31g(d) guess=mix

Stoichiometry C47H67F4NP2
Framework group C1[X(C47H67F4NP2)]
Deg. of freedom 357
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

E(RM062X) = -2967.00477591 A.U.
Dipole moment (field-independent basis, Debye):
X= 0.2381 Y= -5.8785 Z= -0.7317 Tot= 5.9287

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.028119	0.953558	1.143347
2	15	0	0.097704	-0.947718	-0.345290
3	6	0	1.300830	0.104137	0.233668
4	6	0	-1.230425	-0.099213	0.276897
5	6	0	3.383192	-0.086653	-1.117258
6	6	0	4.789359	-1.140885	1.045738
7	6	0	-4.759785	-1.292486	0.991380
8	6	0	3.159854	-0.324540	2.778332
9	6	0	-3.051858	-0.692855	2.728436
10	6	0	5.297000	-1.344851	-0.232874
11	6	0	6.592204	-2.110078	-0.510624
12	6	0	4.593157	-0.767956	-1.281255
13	6	0	-2.684652	-0.352134	0.140995
14	6	0	-4.535400	-0.911174	-1.331619
15	6	0	0.224740	-2.803614	-0.524371
16	6	0	-2.826296	0.782407	3.107459
17	6	0	2.769795	-0.104497	0.176991
18	6	0	-3.492516	-0.781139	1.248860
19	6	0	-5.291725	-1.419034	-0.291737
20	6	0	1.950286	-1.176801	3.194954
21	6	0	-2.651704	0.261836	-2.462781
22	6	0	3.556537	-0.530777	1.295042
23	6	0	7.611611	-1.175501	-1.183342
24	6	0	-4.132337	-1.197629	3.702985
25	6	0	2.122848	1.967898	-2.049196
26	6	0	4.066463	1.110980	-3.255579
27	6	0	2.905097	1.170192	3.035787
28	6	0	-3.269273	-0.327592	-1.158238

29	6	0	2.868669	0.668461	-2.381103
30	6	0	-1.817657	-1.567374	3.014292
31	6	0	-1.901314	-0.830550	-3.242650
32	6	0	7.222225	-2.667549	0.769707
33	6	0	1.977700	-0.208224	-3.274034
34	6	0	4.291241	-0.714871	3.747354
35	6	0	-7.724720	-1.249620	0.276501
36	1	0	-8.715681	-1.698117	0.142108
37	1	0	-7.759694	-0.218747	-0.090580
38	1	0	-7.512788	-1.218677	1.349761
39	6	0	-3.769912	0.780549	-3.401486
40	6	0	-1.739201	1.481574	-2.258331
41	6	0	-6.665563	-2.062210	-0.487307
42	6	0	6.283732	-3.287585	-1.450738
43	6	0	-1.201813	-3.363333	-0.583421
44	6	0	-7.074533	-2.116815	-1.962873
45	6	0	-6.635670	-3.499748	0.058310
46	6	0	1.020824	-3.164015	-1.783473
47	6	0	0.960690	-3.337305	0.710941
48	1	0	7.504342	-1.867367	1.462471
49	1	0	-4.945953	-0.960920	-2.329251
50	1	0	5.369661	-1.495947	1.883718
51	1	0	-4.474110	1.422255	-2.862767
52	1	0	-1.398683	1.836756	-3.237759
53	1	0	-3.760986	-1.071645	4.725155
54	1	0	2.670827	1.330926	4.094297
55	1	0	1.220180	1.787372	-1.470059
56	1	0	1.832275	2.459672	-2.984678
57	1	0	3.968401	-0.483294	4.767411
58	1	0	5.559943	-3.969944	-0.992177
59	1	0	-5.366465	-1.635366	1.818872
60	1	0	4.519501	-1.785162	3.713924
61	1	0	1.762343	0.317550	-4.212369
62	1	0	7.231162	-0.776698	-2.128971
63	1	0	-5.063953	-0.629364	3.619025
64	1	0	-2.411761	0.856173	4.119398
65	1	0	-4.354411	-2.260536	3.560889
66	1	0	2.471381	-1.155026	-3.520805
67	1	0	5.210756	-0.153289	3.552903
68	1	0	1.083734	-1.019650	2.556944
69	1	0	5.018530	-0.839388	-2.275100
70	1	0	5.865696	-2.942077	-2.401568
71	1	0	2.767086	2.650949	-1.488365
72	1	0	3.708802	1.821938	-4.006958
73	1	0	3.797325	1.754077	2.785697
74	1	0	-4.332403	-0.021396	-3.886809
75	1	0	-1.545466	-0.436656	-4.202496
76	1	0	2.209732	-2.241070	3.165602
77	1	0	-3.781096	1.318807	3.083193
78	1	0	8.130251	-3.225879	0.519469
79	1	0	1.658301	-0.927860	4.222047
80	1	0	-0.960939	-1.303057	2.400902
81	1	0	-8.054981	-2.595575	-2.054642
82	1	0	-2.302569	2.289528	-1.783578
83	1	0	-0.855895	1.275685	-1.658480
84	1	0	1.019354	-0.427423	-2.796686
85	1	0	2.080070	1.567726	2.450478
86	1	0	-7.151490	-1.114585	-2.398098

87	1	0	4.528829	0.283349	-3.800997
88	1	0	-7.614363	-3.975569	-0.071766
89	1	0	-1.523933	-1.467256	4.065839
90	1	0	6.541081	-3.349724	1.290040
91	1	0	7.198032	-3.850908	-1.669319
92	1	0	7.848587	-0.328041	-0.531821
93	1	0	-3.314188	1.370499	-4.202705
94	1	0	-1.027969	-1.193834	-2.693949
95	1	0	-6.390329	-3.521091	1.124820
96	1	0	8.540169	-1.717657	-1.395767
97	1	0	-2.153558	1.301372	2.428837
98	1	0	-6.361377	-2.698274	-2.557349
99	1	0	-2.557126	-1.685994	-3.442824
100	1	0	-2.059578	-2.621733	2.830756
101	1	0	-5.887808	-4.099113	-0.471666
102	1	0	4.837778	1.605539	-2.656678
103	1	0	1.063633	-4.425168	0.608703
104	1	0	0.404306	-3.131022	1.629975
105	1	0	1.961804	-2.901699	0.800987
106	1	0	-1.137375	-4.456010	-0.653061
107	1	0	-1.757689	-2.998719	-1.452517
108	1	0	-1.773191	-3.105566	0.313990
109	1	0	1.106841	-4.255942	-1.836918
110	1	0	0.529897	-2.818896	-2.698526
111	1	0	2.031980	-2.743291	-1.747512
112	6	0	-0.179293	2.716009	0.590541
113	6	0	0.935051	3.543851	0.496027
114	6	0	-1.404326	3.343513	0.395264
115	6	0	0.782603	4.881621	0.157059
116	6	0	-1.448606	4.691949	0.062268
117	7	0	-0.382479	5.447054	-0.056619
118	9	0	2.162148	3.064796	0.716754
119	9	0	1.867830	5.636184	0.042848
120	9	0	-2.550893	2.666376	0.499505
121	9	0	-2.631751	5.252073	-0.155346

Rotational constants (GHZ): 0.0709886 0.0376809 0.0329521

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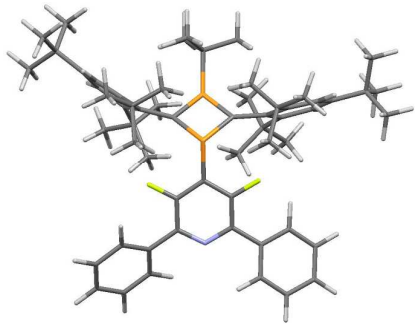

opt m062x/6-31g(d) guess=mix
Stoichiometry C59H77F2NP2
Framework group C1[X(C59H77F2NP2)]
Deg. of freedom 417
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

E(RM062X) = -3230.52095180 A.U.
Dipole moment (field-independent basis, Debye):
X= 0.4469 Y= -2.9137 Z= -1.4250 Tot= 3.2741

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.101310	-0.014036	1.217986
2	15	0	0.424510	-1.779195	-0.409145
3	6	0	1.501379	-0.624547	0.225305
4	6	0	-0.979060	-1.156612	0.302872
5	6	0	3.566078	-0.520305	-1.157652
6	6	0	5.105647	-1.584108	0.908399
7	6	0	-4.410269	-2.636715	0.973846
8	6	0	3.446143	-1.028067	2.713986
9	6	0	-2.658714	-2.192679	2.709212
10	6	0	5.597985	-1.666004	-0.389729
11	6	0	6.942530	-2.305178	-0.740939
12	6	0	4.825308	-1.083910	-1.385766
13	6	0	-2.407919	-1.523167	0.160673
14	6	0	-4.299226	-1.988410	-1.296991
15	6	0	0.783107	-3.586746	-0.726844
16	6	0	-2.569332	-0.772153	3.295437
17	6	0	2.983088	-0.679727	0.141784
18	6	0	-3.147101	-2.116390	1.239965
19	6	0	-4.999420	-2.624625	-0.288096
20	6	0	2.345586	-2.033906	3.087108
21	6	0	-2.471159	-0.689033	-2.383347
22	6	0	3.830777	-1.100302	1.216063
23	6	0	7.867559	-1.253232	-1.375823
24	6	0	-3.646721	-2.944915	3.622163
25	6	0	2.143555	1.497244	-1.907701
26	6	0	4.103046	0.859878	-3.224720
27	6	0	3.031128	0.410472	3.065402
28	6	0	-3.040165	-1.394174	-1.112796
29	6	0	2.963069	0.279154	-2.354007
30	6	0	-1.331432	-2.958100	2.854020
31	6	0	-1.654642	-1.687371	-3.222863
32	6	0	7.647197	-2.885224	0.489271
33	6	0	2.107783	-0.590503	-3.288175
34	6	0	4.632805	-1.345839	3.642256
35	6	0	-7.405409	-2.567817	0.399744
36	1	0	-8.393425	-3.023634	0.267996
37	1	0	-7.478178	-1.505744	0.143386
38	1	0	-7.139687	-2.640527	1.459049

39	6	0	-3.616206	-0.193470	-3.300815
40	6	0	-1.638778	0.576716	-2.119590
41	6	0	-6.370184	-3.271993	-0.493389
42	6	0	6.704164	-3.445873	-1.744888
43	6	0	-0.563171	-4.315017	-0.818318
44	6	0	-6.844157	-3.175947	-1.946921
45	6	0	-6.294196	-4.759153	-0.108490
46	6	0	1.594902	-3.747231	-2.016609
47	6	0	1.600969	-4.120315	0.455664
48	1	0	7.879406	-2.108013	1.225348
49	1	0	-4.752755	-1.943993	-2.275529
50	1	0	5.731974	-1.939294	1.712828
51	1	0	-4.357484	0.383943	-2.738431
52	1	0	-1.281205	0.969468	-3.078688
53	1	0	-3.226096	-2.978476	4.632184
54	1	0	2.785861	0.478036	4.131528
55	1	0	1.261247	1.211770	-1.340152
56	1	0	1.810025	2.046879	-2.795337
57	1	0	4.309593	-1.200393	4.678147
58	1	0	6.046763	-4.208811	-1.313973
59	1	0	-4.968631	-3.098542	1.776458
60	1	0	4.970768	-2.383130	3.550372
61	1	0	1.823417	-0.010158	-4.174582
62	1	0	7.435758	-0.832997	-2.289634
63	1	0	-4.617441	-2.443648	3.689523
64	1	0	-2.245898	-0.818933	4.341903
65	1	0	-3.805954	-3.978207	3.295610
66	1	0	2.662880	-1.473253	-3.625071
67	1	0	5.484527	-0.681780	3.461703
68	1	0	1.463511	-1.940772	2.457644
69	1	0	5.233255	-1.053215	-2.388913
70	1	0	6.236822	-3.078816	-2.664299
71	1	0	2.749185	2.171143	-1.295029
72	1	0	3.676946	1.586184	-3.923772
73	1	0	3.854545	1.101871	2.854522
74	1	0	-4.131086	-1.002773	-3.825555
75	1	0	-1.338515	-1.222017	-4.164543
76	1	0	2.724153	-3.058402	2.997230
77	1	0	-3.553027	-0.292012	3.257155
78	1	0	8.591494	-3.350080	0.187068
79	1	0	2.033788	-1.876861	4.126570
80	1	0	-0.529103	-2.529283	2.260806
81	1	0	-7.821150	-3.659705	-2.048619
82	1	0	-2.262897	1.351447	-1.662706
83	1	0	-0.769635	0.416261	-1.487473
84	1	0	1.185034	-0.919921	-2.803978
85	1	0	2.165570	0.749206	2.503018
86	1	0	-6.952886	-2.134283	-2.268161
87	1	0	4.608823	0.101291	-3.829383
88	1	0	-7.271201	-5.236996	-0.244046
89	1	0	-1.014279	-2.954127	3.903534
90	1	0	7.036430	-3.651708	0.978539
91	1	0	7.654049	-3.921163	-2.015302
92	1	0	8.048816	-0.428579	-0.678761
93	1	0	-3.192185	0.458943	-4.070265
94	1	0	-0.751533	-2.016392	-2.702435
95	1	0	-5.998591	-4.891055	0.937157
96	1	0	8.832416	-1.703827	-1.635893

97	1	0	-1.870240	-0.132336	2.761585
98	1	0	-6.149519	-3.676561	-2.630313
99	1	0	-2.252520	-2.574935	-3.460534
100	1	0	-1.467088	-4.003207	2.548187
101	1	0	-5.564108	-5.283679	-0.733829
102	1	0	4.852575	1.372666	-2.613604
103	1	0	1.842762	-5.173065	0.261102
104	1	0	1.036111	-4.066935	1.390768
105	1	0	2.538712	-3.567390	0.578337
106	1	0	-0.365947	-5.385921	-0.949828
107	1	0	-1.165075	-3.975294	-1.666239
108	1	0	-1.155336	-4.180335	0.092307
109	1	0	1.804153	-4.813741	-2.163830
110	1	0	1.053759	-3.384404	-2.896111
111	1	0	2.552211	-3.217903	-1.950168
112	6	0	-0.303590	1.742375	0.802499
113	6	0	0.666399	2.732191	0.736169
114	6	0	-1.612245	2.183895	0.663121
115	6	0	0.345282	4.066369	0.469050
116	6	0	-1.919009	3.511823	0.352283
117	7	0	-0.929484	4.405236	0.268192
118	9	0	1.946886	2.368205	0.911778
119	9	0	-2.592634	1.280031	0.817189
120	6	0	1.363617	5.141774	0.344720
121	6	0	1.080267	6.233479	-0.484379
122	6	0	2.576283	5.115879	1.042643
123	6	0	1.994795	7.269628	-0.623969
124	1	0	0.133117	6.253377	-1.013191
125	6	0	3.486223	6.159691	0.905180
126	1	0	2.807624	4.290859	1.705501
127	6	0	3.202853	7.235568	0.069486
128	1	0	1.764313	8.106337	-1.276449
129	1	0	4.419813	6.130709	1.458548
130	1	0	3.918510	8.044755	-0.039370
131	6	0	-3.300391	4.007113	0.107094
132	6	0	-3.545269	5.379441	0.242915
133	6	0	-4.349542	3.170017	-0.294282
134	6	0	-4.806976	5.901920	-0.008541
135	1	0	-2.726666	6.024478	0.542999
136	6	0	-5.610192	3.700498	-0.552415
137	1	0	-4.190869	2.104922	-0.412206
138	6	0	-5.845961	5.063840	-0.408104
139	1	0	-4.980493	6.967407	0.108355
140	1	0	-6.411158	3.039455	-0.869280
141	1	0	-6.832575	5.472269	-0.605165

Rotational constants (GHZ): 0.0440388 0.0325613 0.0232889

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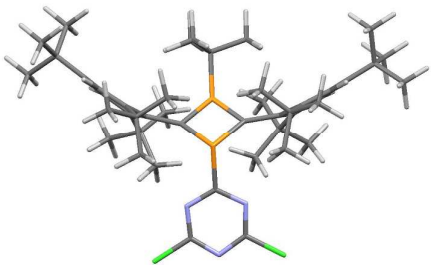


opt=tight m062x/6-31g(d) guess=mix

Stoichiometry C45H67Cl2N3P2
Framework group C1[X(C45H67Cl2N3P2)]
Deg. of freedom 351
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

E(RM062X) = -3521.40394791 A.U.
Dipole moment (field-independent basis, Debye):
X= 0.1865 Y= -4.9010 Z= -0.5793 Tot= 4.9386

Standard orientation:

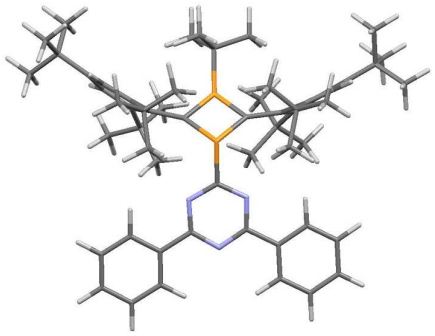
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.006168	0.974760	1.108657
2	15	0	0.083156	-0.960132	-0.338002
3	6	0	1.302715	0.098322	0.207669
4	6	0	-1.227042	-0.088877	0.305434
5	6	0	3.378037	-0.285109	-1.107649
6	6	0	4.713837	-1.240082	1.144507
7	6	0	-4.675358	-1.439457	1.036108
8	6	0	3.125679	-0.122576	2.757158
9	6	0	-3.087924	-0.508135	2.751993
10	6	0	5.194946	-1.602421	-0.111142
11	6	0	6.426795	-2.485665	-0.316974
12	6	0	4.536246	-1.062157	-1.209656
13	6	0	-2.671494	-0.376717	0.170800
14	6	0	-4.401323	-1.223162	-1.305329
15	6	0	0.205793	-2.821933	-0.426475
16	6	0	-2.873030	1.005073	2.953894
17	6	0	2.759731	-0.171931	0.175472
18	6	0	-3.480607	-0.777079	1.285892
19	6	0	-5.130461	-1.741129	-0.250945
20	6	0	1.920952	-0.940218	3.255910
21	6	0	-2.666539	0.163360	-2.438999
22	6	0	3.528587	-0.525142	1.325271
23	6	0	7.520949	-1.687643	-1.046224
24	6	0	-4.198521	-0.899326	3.742707
25	6	0	2.287479	1.829287	-2.063955
26	6	0	4.184800	0.810612	-3.241894
27	6	0	2.881817	1.401555	2.797068
28	6	0	-3.219658	-0.481241	-1.135641
29	6	0	2.937307	0.476378	-2.390513
30	6	0	-1.861629	-1.344537	3.163612
31	6	0	-1.973952	-0.890090	-3.317755
32	6	0	7.002057	-2.993598	1.008766
33	6	0	1.994841	-0.338603	-3.288649
34	6	0	4.248458	-0.377441	3.779220
35	6	0	-7.587328	-1.848654	0.229300
36	1	0	-8.504313	-2.437388	0.111084
37	1	0	-7.746189	-0.866946	-0.228609

38	1	0	-7.420922	-1.697962	1.300470
39	6	0	-3.853165	0.743298	-3.249067
40	6	0	-1.728160	1.363251	-2.231516
41	6	0	-6.401950	-2.571219	-0.432835
42	6	0	6.030291	-3.703051	-1.169353
43	6	0	-1.221759	-3.380342	-0.477517
44	6	0	-6.739551	-2.796175	-1.909653
45	6	0	-6.205736	-3.943685	0.233384
46	6	0	1.011436	-3.240045	-1.661148
47	6	0	0.925735	-3.295311	0.843183
48	1	0	7.347746	-2.169055	1.641304
49	1	0	-4.758415	-1.390826	-2.312591
50	1	0	5.269588	-1.545325	2.019905
51	1	0	-4.435932	1.438745	-2.636548
52	1	0	-1.591247	1.872311	-3.192364
53	1	0	-3.889138	-0.597508	4.748913
54	1	0	2.374687	1.685195	3.726391
55	1	0	1.299608	1.714287	-1.624473
56	1	0	2.182498	2.411990	-2.986365
57	1	0	3.937735	0.033558	4.745914
58	1	0	5.252031	-4.288306	-0.667554
59	1	0	-5.276209	-1.769307	1.874553
60	1	0	4.445948	-1.444130	3.926422
61	1	0	1.814622	0.201008	-4.226453
62	1	0	7.176017	-1.329571	-2.021276
63	1	0	-5.143020	-0.393001	3.519304
64	1	0	-2.371488	1.197687	3.909215
65	1	0	-4.375489	-1.979859	3.763704
66	1	0	2.428199	-1.314451	-3.536470
67	1	0	5.181992	0.115533	3.489618
68	1	0	1.075004	-0.911273	2.573637
69	1	0	4.961570	-1.232706	-2.192364
70	1	0	5.645045	-3.399171	-2.147848
71	1	0	2.899532	2.402226	-1.359332
72	1	0	3.895432	1.505111	-4.036735
73	1	0	3.845090	1.922636	2.762435
74	1	0	-4.531235	-0.019610	-3.637300
75	1	0	-1.659274	-0.446934	-4.270347
76	1	0	2.213336	-1.989540	3.380713
77	1	0	-3.843750	1.512856	2.968370
78	1	0	7.860598	-3.644109	0.811710
79	1	0	1.582518	-0.562678	4.228072
80	1	0	-0.986519	-1.142547	2.551305
81	1	0	-7.644274	-3.407692	-1.990224
82	1	0	-2.170072	2.072015	-1.525419
83	1	0	-0.737579	1.090350	-1.868930
84	1	0	1.023700	-0.499451	-2.812299
85	1	0	2.301293	1.780903	1.955818
86	1	0	-6.928235	-1.849841	-2.428000
87	1	0	4.615472	-0.067669	-3.731140
88	1	0	-7.108709	-4.554498	0.119825
89	1	0	-1.599471	-1.136580	4.207717
90	1	0	6.261778	-3.572624	1.571460
91	1	0	6.897968	-4.351920	-1.334689
92	1	0	7.821815	-0.816332	-0.455437
93	1	0	-3.463988	1.290855	-4.113304
94	1	0	-1.078500	-1.291541	-2.830100
95	1	0	-5.997940	-3.844678	1.303378

96	1	0	8.404655	-2.315097	-1.210486
97	1	0	-2.295037	1.474404	2.158872
98	1	0	-5.931880	-3.320942	-2.431235
99	1	0	-2.645458	-1.728893	-3.534983
100	1	0	-2.098585	-2.412452	3.079992
101	1	0	-5.367204	-4.478685	-0.225248
102	1	0	4.963776	1.285996	-2.637227
103	1	0	1.022138	-4.387688	0.799291
104	1	0	0.359036	-3.037879	1.743288
105	1	0	1.929212	-2.862589	0.924360
106	1	0	-1.158625	-4.475027	-0.502426
107	1	0	-1.766585	-3.048761	-1.366881
108	1	0	-1.803535	-3.085631	0.402153
109	1	0	1.087478	-4.334030	-1.670701
110	1	0	0.530429	-2.926061	-2.592873
111	1	0	2.026164	-2.827520	-1.633057
112	6	0	-0.160756	2.714985	0.519384
113	6	0	0.773672	4.682254	0.027452
114	6	0	-1.427080	4.509571	0.110828
115	7	0	-0.389659	5.302279	-0.123600
116	7	0	-1.394702	3.230100	0.437603
117	7	0	0.967343	3.417152	0.352731
118	17	0	-2.990350	5.228391	-0.044004
119	17	0	2.188268	5.639922	-0.239972

Rotational constants (GHZ): 0.0636793 0.0387781 0.0318243

5b



opt m062x/6-31g(d) guess=mix

Stoichiometry C57H77N3P2
Framework group C1[X(C57H77N3P2)]
Deg. of freedom 411
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

E(RM062X) = -3064.20697622 A.U.
Dipole moment (field-independent basis, Debye):
X= -0.1012 Y= -1.0669 Z= -1.0348 Tot= 1.4898

Standard orientation:

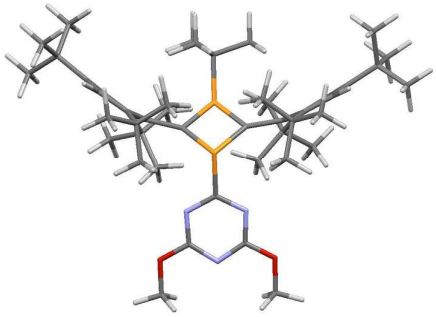
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.059180	0.238349	1.146786
2	15	0	0.136716	-1.643684	-0.375839
3	6	0	1.359551	-0.608046	0.217520
4	6	0	-1.164900	-0.796652	0.327724
5	6	0	3.428721	-0.865335	-1.145835
6	6	0	4.840152	-1.836613	1.053162
7	6	0	-4.621962	-2.126246	1.051622
8	6	0	3.222166	-0.863316	2.727156
9	6	0	-3.014191	-1.248371	2.776352
10	6	0	5.328234	-2.117295	-0.220231
11	6	0	6.609562	-2.914065	-0.472835
12	6	0	4.626518	-1.572891	-1.289401
13	6	0	-2.612341	-1.062996	0.195369
14	6	0	-4.364026	-1.858059	-1.285428
15	6	0	0.259490	-3.505226	-0.483933
16	6	0	-2.785085	0.258419	3.010585
17	6	0	2.821586	-0.829696	0.147922
18	6	0	-3.419593	-1.480062	1.307349
19	6	0	-5.088477	-2.396503	-0.238538
20	6	0	2.039062	-1.724902	3.204250
21	6	0	-2.640608	-0.447850	-2.401916
22	6	0	3.621678	-1.192465	1.274884
23	6	0	7.644290	-2.020406	-1.177229
24	6	0	-4.121802	-1.652553	3.765326
25	6	0	2.231055	1.226205	-2.029584
26	6	0	4.138168	0.319860	-3.272206
27	6	0	2.948615	0.652678	2.832519
28	6	0	-3.176004	-1.127203	-1.108125
29	6	0	2.928817	-0.091661	-2.399964
30	6	0	-1.792461	-2.104037	3.162401
31	6	0	-1.997693	-1.484588	-3.337283
32	6	0	7.230614	-3.438155	0.825655
33	6	0	2.006167	-0.927944	-3.300245
34	6	0	4.358175	-1.137360	3.729380
35	6	0	-7.543909	-2.499953	0.251000
36	1	0	-8.464822	-3.081499	0.127179
37	1	0	-7.699797	-1.509651	-0.189336
38	1	0	-7.370908	-2.368774	1.323741

39	6	0	-3.836958	0.190198	-3.152344
40	6	0	-1.668019	0.721617	-2.185714
41	6	0	-6.365370	-3.216204	-0.429854
42	6	0	6.281806	-4.117799	-1.372081
43	6	0	-1.168091	-4.059843	-0.562312
44	6	0	-6.710787	-3.411631	-1.909082
45	6	0	-6.174514	-4.602162	0.209486
46	6	0	1.076677	-3.897226	-1.719953
47	6	0	0.965621	-4.008751	0.780692
48	1	0	7.532323	-2.619660	1.487993
49	1	0	-4.728720	-2.000570	-2.294073
50	1	0	5.420296	-2.149593	1.909711
51	1	0	-4.373370	0.886455	-2.498831
52	1	0	-1.529634	1.241934	-3.140578
53	1	0	-3.804520	-1.374064	4.775805
54	1	0	2.458052	0.890273	3.783435
55	1	0	1.295499	1.068436	-1.499352
56	1	0	2.015033	1.788429	-2.945463
57	1	0	4.041260	-0.785638	4.717190
58	1	0	5.549093	-4.773255	-0.889145
59	1	0	-5.219252	-2.470783	1.886821
60	1	0	4.586720	-2.204292	3.819579
61	1	0	1.792903	-0.379463	-4.225991
62	1	0	7.267515	-1.644715	-2.133754
63	1	0	-5.064202	-1.135246	3.558255
64	1	0	-2.268891	0.425782	3.962877
65	1	0	-4.306475	-2.732057	3.764595
66	1	0	2.476113	-1.880920	-3.570156
67	1	0	5.275836	-0.603352	3.462564
68	1	0	1.188400	-1.691267	2.528649
69	1	0	5.048231	-1.682970	-2.282110
70	1	0	5.866134	-3.798428	-2.332960
71	1	0	2.872281	1.843602	-1.391090
72	1	0	3.799519	1.033668	-4.029662
73	1	0	3.902009	1.193097	2.798752
74	1	0	-4.553434	-0.539225	-3.535600
75	1	0	-1.710623	-1.015737	-4.286317
76	1	0	2.356758	-2.770655	3.291599
77	1	0	-3.752522	0.772201	3.052900
78	1	0	8.125301	-4.025680	0.594401
79	1	0	1.700162	-1.387991	4.191117
80	1	0	-0.915540	-1.888025	2.557711
81	1	0	-7.618392	-4.017919	-1.997348
82	1	0	-2.077871	1.432961	-1.463371
83	1	0	-0.682248	0.416690	-1.838923
84	1	0	1.048670	-1.137583	-2.816518
85	1	0	2.339420	1.052560	2.021456
86	1	0	-6.897427	-2.454748	-2.408479
87	1	0	4.584767	-0.522272	-3.808818
88	1	0	-7.081740	-5.205429	0.088905
89	1	0	-1.530827	-1.928427	4.212625
90	1	0	6.534763	-4.084176	1.371863
91	1	0	7.187305	-4.701619	-1.573501
92	1	0	7.897861	-1.156986	-0.553372
93	1	0	-3.462012	0.752048	-4.013797
94	1	0	-1.091465	-1.912694	-2.894337
95	1	0	-5.960739	-4.524500	1.280035
96	1	0	8.563053	-2.584762	-1.374788

97	1	0	-2.214956	0.742711	2.218644
98	1	0	-5.907220	-3.929245	-2.443913
99	1	0	-2.688061	-2.307258	-3.556862
100	1	0	-2.036243	-3.167432	3.046835
101	1	0	-5.341310	-5.133223	-0.263065
102	1	0	4.917740	0.800759	-2.672578
103	1	0	1.057581	-5.100815	0.717831
104	1	0	0.394144	-3.764599	1.681501
105	1	0	1.969985	-3.581879	0.877565
106	1	0	-1.109597	-5.153933	-0.615361
107	1	0	-1.703891	-3.702769	-1.447605
108	1	0	-1.756742	-3.785237	0.319432
109	1	0	1.163181	-4.990168	-1.750235
110	1	0	0.599313	-3.569104	-2.648838
111	1	0	2.087524	-3.475542	-1.679043
112	6	0	-0.109962	2.005423	0.646382
113	6	0	0.816979	4.026825	0.288286
114	6	0	-1.434948	3.784130	0.248988
115	7	0	-0.381327	4.593170	0.110874
116	7	0	-1.347905	2.480169	0.538026
117	7	0	1.004270	2.728600	0.557524
118	6	0	-2.792125	4.344795	0.054738
119	6	0	-3.908072	3.502001	0.109383
120	6	0	-2.960990	5.709575	-0.194340
121	6	0	-5.180858	4.026026	-0.085180
122	1	0	-3.763214	2.443174	0.303244
123	6	0	-4.236107	6.228045	-0.384536
124	1	0	-2.085351	6.348254	-0.233683
125	6	0	-5.346694	5.387731	-0.331109
126	1	0	-6.045306	3.370693	-0.045390
127	1	0	-4.365497	7.288869	-0.575230
128	1	0	-6.342000	5.795245	-0.481345
129	6	0	2.021394	4.881971	0.173359
130	6	0	3.290663	4.332118	0.381299
131	6	0	1.894612	6.237558	-0.142696
132	6	0	4.420695	5.133253	0.268807
133	1	0	3.373849	3.279744	0.633456
134	6	0	3.027654	7.034402	-0.253124
135	1	0	0.904172	6.650467	-0.299707
136	6	0	4.291520	6.483942	-0.048609
137	1	0	5.404276	4.703137	0.429708
138	1	0	2.925852	8.086784	-0.499330
139	1	0	5.176040	7.108092	-0.134730

Rotational constants (GHZ): 0.0460090 0.0337654 0.0242685

5c model (OMe)



opt m062x/6-31g(d) guess=mix

Stoichiometry C47H73N3O2P2
Framework group C1[X(C47H73N3O2P2)]
Deg. of freedom 375
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

E(RM062X) = -2831.25727577 A.U.
Dipole moment (field-independent basis, Debye):
X= -0.2711 Y= 1.8122 Z= -1.3833 Tot= 2.2959

Standard orientation:

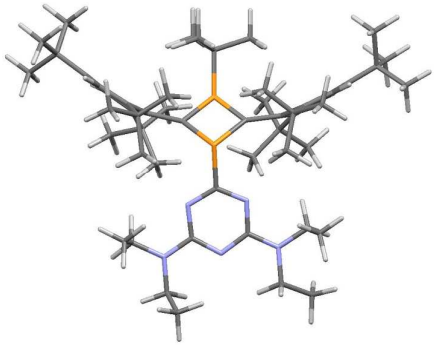
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.011301	0.942841	1.093270
2	15	0	0.068088	-0.989301	-0.368011
3	6	0	1.292289	0.053025	0.209131
4	6	0	-1.235599	-0.110970	0.293369
5	6	0	3.360865	-0.343219	-1.112672
6	6	0	4.696697	-1.302652	1.135976
7	6	0	-4.665158	-1.494903	1.041061
8	6	0	3.124555	-0.168802	2.752382
9	6	0	-3.091866	-0.519542	2.746718
10	6	0	5.168478	-1.675837	-0.120235
11	6	0	6.386869	-2.577147	-0.327583
12	6	0	4.510720	-1.132545	-1.217510
13	6	0	-2.677807	-0.407789	0.166944
14	6	0	-4.393015	-1.296923	-1.302036
15	6	0	0.179789	-2.855857	-0.418982
16	6	0	-2.876140	0.996345	2.929956
17	6	0	2.746356	-0.222329	0.171593
18	6	0	-3.482903	-0.808405	1.284821
19	6	0	-5.111585	-1.821294	-0.243605
20	6	0	1.917875	-0.979402	3.257588
21	6	0	-2.701281	0.140415	-2.437987
22	6	0	3.518868	-0.576375	1.319498
23	6	0	7.487344	-1.801715	-1.071312
24	6	0	-4.202715	-0.898831	3.741683
25	6	0	2.260865	1.766260	-2.079649
26	6	0	4.178724	0.762595	-3.234578
27	6	0	2.886145	1.355854	2.791014
28	6	0	-3.228426	-0.527297	-1.136734
29	6	0	2.924357	0.417964	-2.396784
30	6	0	-1.865686	-1.352665	3.165198
31	6	0	-2.035681	-0.895847	-3.357165
32	6	0	6.964646	-3.082412	0.998138
33	6	0	1.998434	-0.406357	-3.304081
34	6	0	4.251049	-0.427469	3.769358
35	6	0	-7.566934	-1.978493	0.232522
36	1	0	-8.470550	-2.588852	0.119749
37	1	0	-7.746207	-1.005926	-0.237338
38	1	0	-7.405812	-1.811206	1.301996

39	6	0	-3.909408	0.742736	-3.198123
40	6	0	-1.750268	1.330018	-2.228392
41	6	0	-6.363785	-2.681518	-0.418374
42	6	0	5.966965	-3.796139	-1.166511
43	6	0	-1.249876	-3.406983	-0.482366
44	6	0	-6.692754	-2.931081	-1.893220
45	6	0	-6.139209	-4.041788	0.263539
46	6	0	0.994236	-3.293094	-1.641631
47	6	0	0.882905	-3.323982	0.860829
48	1	0	7.324392	-2.257376	1.622197
49	1	0	-4.743705	-1.480635	-2.309413
50	1	0	5.252895	-1.610230	2.010341
51	1	0	-4.449622	1.449523	-2.559960
52	1	0	-1.673005	1.885834	-3.170355
53	1	0	-3.897305	-0.576391	4.742853
54	1	0	2.385430	1.641472	3.723439
55	1	0	1.277707	1.649321	-1.630829
56	1	0	2.143549	2.334377	-3.010112
57	1	0	3.947689	-0.011045	4.736177
58	1	0	5.182861	-4.364449	-0.654458
59	1	0	-5.260548	-1.826064	1.883183
60	1	0	4.443036	-1.494857	3.919553
61	1	0	1.831689	0.125510	-4.248894
62	1	0	7.140181	-1.446199	-2.046485
63	1	0	-5.149286	-0.401811	3.505807
64	1	0	-2.355899	1.198413	3.873426
65	1	0	-4.374358	-1.979714	3.782813
66	1	0	2.438285	-1.383143	-3.537004
67	1	0	5.186193	0.058680	3.473040
68	1	0	1.067918	-0.939808	2.581069
69	1	0	4.928306	-1.311967	-2.202282
70	1	0	5.579274	-3.494579	-2.144816
71	1	0	2.867998	2.356550	-1.385640
72	1	0	3.893365	1.458020	-4.030330
73	1	0	3.851428	1.873319	2.751399
74	1	0	-4.620110	-0.006601	-3.552941
75	1	0	-1.738539	-0.430331	-4.304816
76	1	0	2.203250	-2.031294	3.377581
77	1	0	-3.848331	1.500921	2.961510
78	1	0	7.813638	-3.745422	0.800778
79	1	0	1.589832	-0.601531	4.233344
80	1	0	-0.994072	-1.160503	2.544767
81	1	0	-7.583530	-3.563525	-1.969192
82	1	0	-2.136826	2.003271	-1.458175
83	1	0	-0.739099	1.035750	-1.948549
84	1	0	1.020806	-0.566627	-2.840643
85	1	0	2.303098	1.738364	1.953244
86	1	0	-6.900781	-1.995242	-2.423181
87	1	0	4.621056	-0.110960	-3.721962
88	1	0	-7.027689	-4.674611	0.154726
89	1	0	-1.597349	-1.130324	4.204912
90	1	0	6.220487	-3.647353	1.569916
91	1	0	6.823359	-4.460031	-1.331999
92	1	0	7.804892	-0.930180	-0.489571
93	1	0	-3.547495	1.282970	-4.079047
94	1	0	-1.132570	-1.312764	-2.897268
95	1	0	-5.936262	-3.925863	1.332774
96	1	0	8.360613	-2.443409	-1.237081

97	1	0	-2.318185	1.463227	2.119184
98	1	0	-5.871919	-3.443387	-2.406569
99	1	0	-2.714836	-1.726424	-3.582151
100	1	0	-2.105805	-2.421082	3.097664
101	1	0	-5.287165	-4.562360	-0.186806
102	1	0	4.947756	1.240785	-2.619429
103	1	0	0.970481	-4.417812	0.829662
104	1	0	0.310680	-3.052225	1.753075
105	1	0	1.889176	-2.898941	0.947118
106	1	0	-1.194255	-4.502414	-0.500675
107	1	0	-1.782472	-3.076311	-1.379773
108	1	0	-1.839869	-3.102966	0.388724
109	1	0	1.065234	-4.387666	-1.639785
110	1	0	0.522733	-2.985772	-2.580665
111	1	0	2.010868	-2.885050	-1.610362
112	6	0	-0.135152	2.700158	0.538819
113	6	0	0.855902	4.652529	0.105145
114	6	0	-1.372891	4.521580	0.169930
115	7	0	-0.305075	5.293887	-0.030517
116	7	0	-1.359724	3.221900	0.460441
117	7	0	1.012141	3.363548	0.398644
118	8	0	-2.580899	5.061269	0.074021
119	8	0	1.984888	5.328768	-0.062854
120	6	0	-2.652734	6.449413	-0.237105
121	1	0	-2.197825	6.650324	-1.209857
122	1	0	-3.715908	6.683625	-0.256126
123	1	0	-2.142073	7.042532	0.525098
124	6	0	1.875122	6.711736	-0.385053
125	1	0	2.900697	7.067814	-0.469642
126	1	0	1.342925	6.846846	-1.329647
127	1	0	1.345285	7.251235	0.403358

Rotational constants (GHZ): 0.0619762 0.0394388 0.0318273

5d



opt m062x/6-31g(d) guess=mix

Stoichiometry C53H87N5P2
Framework group C1[X(C53H87N5P2)]
Deg. of freedom 435
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

E(RM062X) = -3027.31294483 A.U.
Dipole moment (field-independent basis, Debye):
X= -0.6372 Y= 1.3063 Z= -0.6588 Tot= 1.5957

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.081338	0.425897	0.950428
2	15	0	0.331571	-1.611969	-0.344078
3	6	0	1.455354	-0.404374	0.128992
4	6	0	-1.038956	-0.806748	0.284120
5	6	0	3.545153	-0.686790	-1.197226
6	6	0	5.019600	-1.223168	1.105024
7	6	0	-4.361630	-2.374161	1.138613
8	6	0	3.329361	-0.144233	2.635124
9	6	0	-2.868964	-1.167582	2.764886
10	6	0	5.530119	-1.649398	-0.118085
11	6	0	6.868519	-2.375191	-0.264126
12	6	0	4.792305	-1.317060	-1.248395
13	6	0	-2.453800	-1.215870	0.179133
14	6	0	-4.096611	-2.337230	-1.212835
15	6	0	0.619075	-3.453620	-0.178986
16	6	0	-2.797206	0.370209	2.841846
17	6	0	2.929749	-0.517107	0.083140
18	6	0	-3.232163	-1.588639	1.326916
19	6	0	-4.779791	-2.828378	-0.116336
20	6	0	2.236633	-1.035134	3.252753
21	6	0	-2.499627	-0.899109	-2.470648
22	6	0	3.754706	-0.647366	1.241999
23	6	0	7.826980	-1.529519	-1.119771
24	6	0	-3.940360	-1.581216	3.789410
25	6	0	2.232881	1.196435	-2.332353
26	6	0	4.186647	0.247319	-3.465548
27	6	0	2.915144	1.338840	2.520484
28	6	0	-2.988760	-1.476660	-1.111489
29	6	0	3.002385	-0.117405	-2.539499
30	6	0	-1.568938	-1.843191	3.239503
31	6	0	-1.780500	-1.980635	-3.293478
32	6	0	7.536223	-2.635377	1.090080
33	6	0	2.136249	-1.115178	-3.324366
34	6	0	4.489337	-0.159099	3.647206
35	6	0	-7.216381	-3.140105	0.383662
36	1	0	-8.070914	-3.823303	0.315403
37	1	0	-7.468009	-2.218458	-0.151234
38	1	0	-7.070693	-2.889142	1.438882

39	6	0	-3.740375	-0.433000	-3.273528
40	6	0	-1.612139	0.353027	-2.388546
41	6	0	-5.962116	-3.792574	-0.221591
42	6	0	6.632828	-3.729553	-0.953741
43	6	0	-0.752717	-4.139117	-0.200825
44	6	0	-6.270962	-4.172049	-1.673210
45	6	0	-5.633319	-5.079280	0.554303
46	6	0	1.494537	-3.938790	-1.340019
47	6	0	1.332736	-3.718116	1.151154
48	1	0	7.772938	-1.700807	1.609845
49	1	0	-4.427229	-2.629894	-2.201038
50	1	0	5.620529	-1.364667	1.992529
51	1	0	-4.315289	0.299865	-2.697030
52	1	0	-1.548539	0.801163	-3.386951
53	1	0	-3.663789	-1.169820	4.766036
54	1	0	2.395662	1.665209	3.429496
55	1	0	1.318950	1.069537	-1.758145
56	1	0	1.970451	1.620256	-3.308727
57	1	0	4.147132	0.313210	4.574608
58	1	0	5.961100	-4.355302	-0.356361
59	1	0	-4.932280	-2.686166	2.004523
60	1	0	4.812531	-1.174621	3.898539
61	1	0	1.903814	-0.706823	-4.315748
62	1	0	7.424621	-1.354952	-2.122694
63	1	0	-4.928971	-1.187948	3.530849
64	1	0	-2.335722	0.685969	3.785105
65	1	0	-4.013286	-2.668605	3.899400
66	1	0	2.663977	-2.065828	-3.464027
67	1	0	5.355402	0.403792	3.284058
68	1	0	1.384101	-1.179290	2.595157
69	1	0	5.224048	-1.532121	-2.219579
70	1	0	6.183441	-3.602272	-1.943657
71	1	0	2.854941	1.923167	-1.798350
72	1	0	3.806121	0.834373	-4.307565
73	1	0	3.816258	1.953790	2.406935
74	1	0	-4.412977	-1.246450	-3.554061
75	1	0	-1.499465	-1.586431	-4.277715
76	1	0	2.654922	-2.022464	3.481804
77	1	0	-3.812908	0.782420	2.805689
78	1	0	8.474689	-3.179148	0.938881
79	1	0	1.871339	-0.594009	4.187860
80	1	0	-0.709590	-1.579017	2.628914
81	1	0	-7.110364	-4.874783	-1.699240
82	1	0	-2.039356	1.089712	-1.703260
83	1	0	-0.592394	0.148544	-2.065742
84	1	0	1.187651	-1.316006	-2.821548
85	1	0	2.281595	1.564796	1.661975
86	1	0	-6.550058	-3.295734	-2.268284
87	1	0	4.681593	-0.630828	-3.890992
88	1	0	-6.469506	-5.785496	0.493563
89	1	0	-1.352760	-1.550506	4.273968
90	1	0	6.897597	-3.240482	1.742473
91	1	0	7.581821	-4.263858	-1.079133
92	1	0	8.001855	-0.554534	-0.653073
93	1	0	-3.410976	0.045107	-4.201788
94	1	0	-0.861580	-2.310888	-2.795007
95	1	0	-5.441847	-4.872533	1.611917
96	1	0	8.791636	-2.038890	-1.227675

97	1	0	-2.248418	0.826483	2.017807
98	1	0	-5.413145	-4.655787	-2.152609
99	1	0	-2.417400	-2.859768	-3.445492
100	1	0	-1.689203	-2.933460	3.214499
101	1	0	-4.742217	-5.562161	0.138970
102	1	0	4.937453	0.846675	-2.940476
103	1	0	1.509484	-4.797518	1.246366
104	1	0	0.724064	-3.394823	2.001160
105	1	0	2.298763	-3.203609	1.196678
106	1	0	-0.599494	-5.221170	-0.103572
107	1	0	-1.295527	-3.955067	-1.133953
108	1	0	-1.385371	-3.802635	0.627269
109	1	0	1.674269	-5.014131	-1.218529
110	1	0	1.011193	-3.783698	-2.310224
111	1	0	2.465402	-3.429834	-1.348976
112	6	0	-0.278385	2.116018	0.297548
113	6	0	0.390531	4.191651	-0.223388
114	6	0	-1.815492	3.677468	-0.210717
115	7	0	-0.871257	4.604964	-0.414210
116	7	0	-1.566169	2.408798	0.184252
117	7	0	0.750438	2.935708	0.134788
118	7	0	-3.114031	4.020926	-0.418984
119	7	0	1.381445	5.095758	-0.401693
120	6	0	2.761063	4.736425	-0.083758
121	1	0	2.922937	3.704938	-0.401006
122	1	0	3.408860	5.381821	-0.684957
123	6	0	3.089171	4.872186	1.400743
124	1	0	2.980931	5.905666	1.742271
125	1	0	2.421489	4.235063	1.988258
126	1	0	4.119537	4.555964	1.591435
127	6	0	1.049403	6.474686	-0.745153
128	1	0	0.289747	6.453162	-1.530977
129	1	0	1.954754	6.922426	-1.166056
130	6	0	0.542392	7.302311	0.433772
131	1	0	-0.362523	6.848303	0.844988
132	1	0	1.293335	7.370648	1.225608
133	1	0	0.301596	8.317837	0.103865
134	6	0	-3.446892	5.429413	-0.632442
135	1	0	-3.482115	5.956842	0.333052
136	1	0	-2.625961	5.869712	-1.198270
137	6	0	-4.758295	5.624943	-1.382056
138	1	0	-5.627948	5.320196	-0.792783
139	1	0	-4.878077	6.684918	-1.621807
140	1	0	-4.758245	5.059451	-2.318680
141	6	0	-4.174228	3.109524	0.008515
142	1	0	-3.791959	2.091493	-0.070794
143	1	0	-5.007806	3.206395	-0.692239
144	6	0	-4.632008	3.389497	1.437243
145	1	0	-5.417018	2.686694	1.732269
146	1	0	-3.790908	3.275512	2.128313
147	1	0	-5.030077	4.405046	1.540177

Rotational constants (GHZ): 0.0480273 0.0354839 0.0259859

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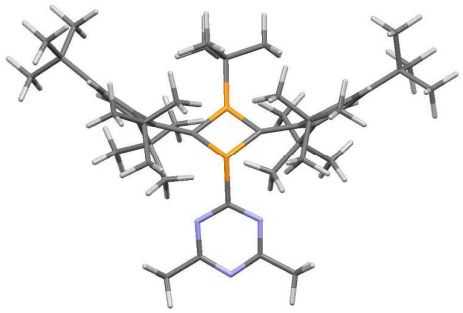


opt m062x/6-31g(d) guess=mix

Stoichiometry C47H73N3P2
Framework group C1[X(C47H73N3P2)]
Deg. of freedom 369
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

E(RM062X) = -2680.87126377 A.U.
Dipole moment (field-independent basis, Debye):
X= -0.1037 Y= -1.4298 Z= -0.8610 Tot= 1.6723

Standard orientation:

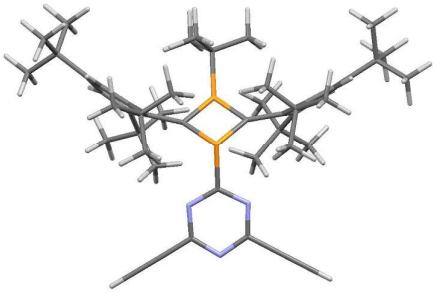
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.010943	1.240445	1.050765
2	15	0	0.054781	-0.733528	-0.356272
3	6	0	1.285607	0.320236	0.187957
4	6	0	-1.242188	0.168434	0.286198
5	6	0	3.350681	-0.139954	-1.116875
6	6	0	4.674150	-1.042151	1.162262
7	6	0	-4.684086	-1.164173	1.066815
8	6	0	3.115212	0.164366	2.739028
9	6	0	-3.103774	-0.156083	2.746627
10	6	0	5.139384	-1.464617	-0.080853
11	6	0	6.341753	-2.393398	-0.257799
12	6	0	4.489785	-0.947638	-1.195700
13	6	0	-2.686939	-0.117876	0.164876
14	6	0	-4.410924	-1.029024	-1.280513
15	6	0	0.158553	-2.601682	-0.352904
16	6	0	-2.878933	1.362860	2.888329
17	6	0	2.736825	0.028853	0.162360
18	6	0	-3.496156	-0.481538	1.292599
19	6	0	-5.133804	-1.519708	-0.208980
20	6	0	1.902554	-0.619870	3.271198
21	6	0	-2.703854	0.357240	-2.455460
22	6	0	3.505570	-0.295301	1.321327
23	6	0	7.456238	-1.663895	-1.026310
24	6	0	-4.217665	-0.500138	3.751205
25	6	0	2.286923	1.958253	-2.140438
26	6	0	4.185576	0.888229	-3.270520
27	6	0	2.888291	1.691580	2.725146
28	6	0	-3.238480	-0.267050	-1.135599
29	6	0	2.925981	0.590271	-2.422812
30	6	0	-1.882989	-0.984755	3.188880
31	6	0	-2.048551	-0.712230	-3.343614
32	6	0	6.909936	-2.865657	1.084129
33	6	0	1.984503	-0.241571	-3.306886
34	6	0	4.240287	-0.067448	3.763979
35	6	0	-7.589233	-1.649685	0.277074
36	1	0	-8.496665	-2.257113	0.181076
37	1	0	-7.764827	-0.686976	-0.214047
38	1	0	-7.423995	-1.459354	1.342040

39	6	0	-3.904688	0.949719	-3.234671
40	6	0	-1.740771	1.542599	-2.280057
41	6	0	-6.392487	-2.374641	-0.361416
42	6	0	5.898404	-3.631340	-1.056158
43	6	0	-1.273764	-3.147414	-0.401499
44	6	0	-6.727343	-2.654377	-1.829592
45	6	0	-6.174676	-3.720996	0.349594
46	6	0	0.970753	-3.076770	-1.562855
47	6	0	0.858661	-3.036095	0.940092
48	1	0	7.287165	-2.027786	1.680177
49	1	0	-4.763773	-1.236353	-2.282521
50	1	0	5.227009	-1.327717	2.046180
51	1	0	-4.440222	1.679101	-2.617905
52	1	0	-1.655451	2.070145	-3.237271
53	1	0	-3.909622	-0.153025	4.743271
54	1	0	2.388985	2.012994	3.646564
55	1	0	1.294813	1.870993	-1.704505
56	1	0	2.197012	2.514812	-3.080885
57	1	0	3.940828	0.383358	4.716458
58	1	0	5.101974	-4.166184	-0.527354
59	1	0	-5.281257	-1.469006	1.917434
60	1	0	4.424694	-1.130404	3.949905
61	1	0	1.823321	0.268905	-4.264304
62	1	0	7.115560	-1.333126	-2.012425
63	1	0	-5.160719	-0.002808	3.502191
64	1	0	-2.366753	1.588839	3.830728
65	1	0	-4.397158	-1.578159	3.821638
66	1	0	2.409062	-1.230261	-3.516377
67	1	0	5.178925	0.401188	3.450816
68	1	0	1.054564	-0.602020	2.591180
69	1	0	4.904521	-1.165309	-2.173941
70	1	0	5.518619	-3.355074	-2.045023
71	1	0	2.898229	2.542471	-1.444378
72	1	0	3.912211	1.560728	-4.089806
73	1	0	3.858139	2.199428	2.669594
74	1	0	-4.622265	0.197809	-3.569658
75	1	0	-1.743175	-0.277578	-4.303204
76	1	0	2.182419	-1.667761	3.431715
77	1	0	-3.848570	1.873831	2.896334
78	1	0	7.744879	-3.552261	0.909031
79	1	0	1.573926	-0.204128	4.231217
80	1	0	-1.010686	-0.818121	2.561903
81	1	0	-7.623126	-3.281360	-1.889252
82	1	0	-2.122645	2.241239	-1.530184
83	1	0	-0.733426	1.247791	-1.987488
84	1	0	1.006320	-0.375893	-2.836838
85	1	0	2.307988	2.048750	1.874010
86	1	0	-6.929922	-1.729104	-2.379923
87	1	0	4.613917	-0.008005	-3.728082
88	1	0	-7.067285	-4.350421	0.256784
89	1	0	-1.611954	-0.733705	4.221318
90	1	0	6.154906	-3.396085	1.674441
91	1	0	6.741119	-4.317946	-1.197144
92	1	0	7.791780	-0.780859	-0.472653
93	1	0	-3.536285	1.461681	-4.129617
94	1	0	-1.152435	-1.128230	-2.869479
95	1	0	-5.968405	-3.583015	1.415577
96	1	0	8.316094	-2.328154	-1.171409

97	1	0	-2.309223	1.801525	2.069933
98	1	0	-5.912008	-3.184397	-2.333621
99	1	0	-2.738231	-1.539546	-3.546844
100	1	0	-2.131395	-2.052775	3.153693
101	1	0	-5.326985	-4.256554	-0.091291
102	1	0	4.962630	1.373598	-2.671184
103	1	0	0.939333	-4.130846	0.941879
104	1	0	0.287931	-2.734074	1.823494
105	1	0	1.867562	-2.615133	1.014025
106	1	0	-1.223556	-4.243189	-0.391493
107	1	0	-1.805156	-2.837509	-1.306973
108	1	0	-1.861775	-2.818587	0.461893
109	1	0	1.038909	-4.171006	-1.528993
110	1	0	0.498905	-2.795724	-2.510018
111	1	0	1.988586	-2.670842	-1.545040
112	6	0	-0.139456	2.977770	0.440799
113	6	0	0.852636	4.924692	-0.099882
114	6	0	-1.400656	4.791117	-0.000141
115	7	0	-0.324791	5.541028	-0.251954
116	7	0	-1.361943	3.502093	0.355650
117	7	0	1.000405	3.646088	0.257899
118	6	0	-2.754081	5.417180	-0.145794
119	1	0	-2.663284	6.497789	-0.253749
120	1	0	-3.246932	5.005778	-1.033294
121	1	0	-3.375014	5.166413	0.717370
122	6	0	2.098616	5.708692	-0.378439
123	1	0	2.422787	5.508673	-1.406015
124	1	0	1.907185	6.777297	-0.277264
125	1	0	2.899817	5.390027	0.290788

Rotational constants (GHZ): 0.0744682 0.0399368 0.0351849

5g model (H)



opt m062x/6-31g(d) guess=mix

Stoichiometry C49H69N3P2
Framework group C1[X(C49H69N3P2)]
Deg. of freedom 363
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

E(RM062X) = -2754.48919255 A.U.
Dipole moment (field-independent basis, Debye):
X= -0.0538 Y= -2.0127 Z= -0.9103 Tot= 2.2097

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.010600	1.077102	1.100838
2	15	0	0.059213	-0.856766	-0.355185
3	6	0	1.288922	0.184159	0.208296
4	6	0	-1.240786	0.027665	0.299581
5	6	0	3.358865	-0.227931	-1.107389
6	6	0	4.684534	-1.188395	1.147596
7	6	0	-4.686472	-1.322368	1.036341
8	6	0	3.112880	-0.043391	2.756594
9	6	0	-3.104076	-0.373108	2.748069
10	6	0	5.157915	-1.566297	-0.106485
11	6	0	6.373604	-2.472388	-0.308664
12	6	0	4.505480	-1.022556	-1.206857
13	6	0	-2.685770	-0.255528	0.168348
14	6	0	-4.410169	-1.117101	-1.305796
15	6	0	0.162089	-2.722388	-0.420068
16	6	0	-2.879259	1.140388	2.938306
17	6	0	2.742040	-0.101123	0.175371
18	6	0	-3.495856	-0.651916	1.284117
19	6	0	-5.136644	-1.635979	-0.250046
20	6	0	1.902452	-0.849266	3.260661
21	6	0	-2.692868	0.292275	-2.438100
22	6	0	3.509347	-0.456530	1.326017
23	6	0	7.478950	-1.702005	-1.050464
24	6	0	-4.218612	-0.749535	3.740010
25	6	0	2.287753	1.892626	-2.076666
26	6	0	4.185936	0.857509	-3.237701
27	6	0	2.880724	1.482612	2.790551
28	6	0	-3.234744	-0.364913	-1.137030
29	6	0	2.930148	0.534260	-2.393830
30	6	0	-1.883555	-1.214885	3.165718
31	6	0	-2.025459	-0.754189	-3.344317
32	6	0	6.945522	-2.977420	1.019701
33	6	0	1.988401	-0.277404	-3.295995
34	6	0	4.235654	-0.302938	3.777505
35	6	0	-7.593868	-1.762374	0.225366
36	1	0	-8.505444	-2.360014	0.109282
37	1	0	-7.760395	-0.785076	-0.239314
38	1	0	-7.430762	-1.603102	1.295786

39	6	0	-3.888693	0.897445	-3.215358
40	6	0	-1.737109	1.477926	-2.227845
41	6	0	-6.400446	-2.478193	-0.429525
42	6	0	5.951649	-3.691205	-1.146820
43	6	0	-1.270690	-3.265712	-0.482045
44	6	0	-6.732703	-2.715245	-1.905669
45	6	0	-6.194068	-3.844921	0.245275
46	6	0	0.972975	-3.158839	-1.645135
47	6	0	0.865279	-3.196887	0.857880
48	1	0	7.307205	-2.152763	1.643142
49	1	0	-4.763201	-1.292021	-2.313683
50	1	0	5.237322	-1.495959	2.024115
51	1	0	-4.437932	1.604654	-2.585411
52	1	0	-1.633540	2.017394	-3.176387
53	1	0	-3.911121	-0.436828	4.743549
54	1	0	2.373122	1.773086	3.717584
55	1	0	1.301356	1.787572	-1.631703
56	1	0	2.181520	2.466523	-3.004555
57	1	0	3.931215	0.117156	4.742357
58	1	0	5.164378	-4.256224	-0.635993
59	1	0	-5.286567	-1.650422	1.876227
60	1	0	4.423495	-1.370510	3.931087
61	1	0	1.822673	0.257613	-4.239110
62	1	0	7.136261	-1.347317	-2.027523
63	1	0	-5.160871	-0.242981	3.507416
64	1	0	-2.369099	1.336326	3.888419
65	1	0	-4.399213	-1.829180	3.773287
66	1	0	2.414639	-1.259173	-3.532781
67	1	0	5.173252	0.179090	3.482346
68	1	0	1.055453	-0.813309	2.580187
69	1	0	4.925766	-1.205443	-2.189686
70	1	0	5.567849	-3.390072	-2.126786
71	1	0	2.903975	2.470517	-1.379873
72	1	0	3.907454	1.553405	-4.035335
73	1	0	3.848381	1.995964	2.757698
74	1	0	-4.594486	0.149586	-3.582688
75	1	0	-1.719724	-0.298150	-4.293762
76	1	0	2.185992	-1.900833	3.387311
77	1	0	-3.847532	1.652842	2.958405
78	1	0	7.792226	-3.644323	0.825961
79	1	0	1.570095	-0.466155	4.232832
80	1	0	-1.008416	-1.024094	2.549803
81	1	0	-7.631772	-3.335356	-1.984765
82	1	0	-2.141153	2.167150	-1.481066
83	1	0	-0.735179	1.183302	-1.916883
84	1	0	1.011436	-0.425822	-2.827428
85	1	0	2.306513	1.864659	1.946355
86	1	0	-6.928428	-1.773824	-2.430377
87	1	0	4.613368	-0.024587	-3.722977
88	1	0	-7.091325	-4.464581	0.133544
89	1	0	-1.617991	-0.999773	4.207589
90	1	0	6.197537	-3.538288	1.590499
91	1	0	6.806252	-4.358165	-1.308761
92	1	0	7.797878	-0.830528	-0.469401
93	1	0	-3.512526	1.437928	-4.089913
94	1	0	-1.127529	-1.172257	-2.875514
95	1	0	-5.989214	-3.737499	1.315022
96	1	0	8.350357	-2.347155	-1.212126

97	1	0	-2.306423	1.603245	2.135644
98	1	0	-5.918957	-3.235715	-2.422054
99	1	0	-2.707739	-1.582896	-3.566541
100	1	0	-2.128800	-2.281664	3.091483
101	1	0	-5.349710	-4.375050	-0.208332
102	1	0	4.964515	1.327155	-2.627971
103	1	0	0.948326	-4.290826	0.822641
104	1	0	0.295110	-2.925970	1.751753
105	1	0	1.873437	-2.776296	0.944179
106	1	0	-1.220342	-4.361293	-0.501197
107	1	0	-1.802671	-2.931980	-1.378572
108	1	0	-1.857950	-2.959664	0.390141
109	1	0	1.037982	-4.253700	-1.646716
110	1	0	0.502292	-2.846216	-2.582712
111	1	0	1.991743	-2.756461	-1.612901
112	6	0	-0.133307	2.826683	0.525052
113	6	0	0.861929	4.779912	0.021317
114	6	0	-1.375454	4.658358	0.117942
115	7	0	-0.303247	5.418030	-0.125027
116	7	0	-1.354311	3.363260	0.448029
117	7	0	1.010187	3.495489	0.357415
118	6	0	2.065815	5.538025	-0.211139
119	6	0	3.076685	6.160304	-0.409076
120	1	0	3.972836	6.713116	-0.586175
121	6	0	-2.668347	5.285305	0.002494
122	6	0	-3.750561	5.802213	-0.097573
123	1	0	-4.710976	6.260324	-0.187465

Rotational constants (GHZ): 0.0672994 0.0389957 0.0328505

DFT calculations of 7

DFT calculations were carried out with Gaussian 09 program package.[S3] The structures were optimize by use of the M06-2X Hamiltonian accounting for the "medium-range" correlations[S4,S5] and the 6-31G(d) basis sets. AIM[S6] calculations were performed with AIMAll software package.[S7]

Optimized structure of 7

opt m062x/6-31g(d) guess=mix

Stoichiometry C50H68P2
Framework group CI[X(C50H68P2)]
Deg. of freedom 177
Full point group CI NOp 2
Largest Abelian subgroup CI NOp 2
Largest concise Abelian subgroup CI NOp 2

E(RM062X) = -2627.92913332 A.U.
Dipole moment (field-independent basis, Debye):
X = 0.0000 Y = 0.0000 Z = 0.0000 Tot = 0.0000

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.101517	0.246685	0.423046
2	6	0	0.254285	0.661885	-1.051256
3	6	0	1.715819	1.635667	-2.833821
4	6	0	2.277194	2.792726	-3.381923
5	6	0	0.584693	1.779404	-1.970745
6	6	0	2.393718	0.293813	-3.231537
7	6	0	1.816396	1.603475	1.401307
8	6	0	1.746796	4.064538	-3.203589
9	6	0	-0.051137	3.057089	-1.878292
10	6	0	2.354157	2.730769	0.766351
11	6	0	0.553793	4.154514	-2.496607
12	6	0	3.419850	-0.167068	-2.179635
13	6	0	1.917901	1.469497	2.789987
14	6	0	-1.384904	3.308063	-1.136537
15	6	0	2.456311	5.277778	-3.808725
16	6	0	-2.501150	2.461682	-1.786142
17	6	0	-1.870360	4.765034	-1.271700
18	6	0	1.372514	-0.822629	-3.496247
19	6	0	3.034417	3.603290	2.915888
20	6	0	3.177335	0.447724	-4.554707
21	6	0	2.952030	3.728313	1.530554
22	6	0	-1.259547	3.083387	0.384758
23	6	0	1.731755	6.589935	-3.492924
24	6	0	2.521686	2.470583	3.543802
25	6	0	2.529563	5.121086	-5.337002

26	6	0	3.881415	5.364517	-3.236934
27	1	0	0.094111	5.126096	-2.397280
28	1	0	3.171913	2.704189	-3.984803
29	1	0	2.942409	-0.519231	-1.264086
30	1	0	-0.488934	3.746510	0.794769
31	1	0	2.303091	2.834955	-0.314796
32	1	0	-1.199407	5.472745	-0.773521
33	1	0	4.096241	1.030349	-4.437413
34	1	0	-2.209412	1.431818	-1.990319
35	1	0	1.509645	0.588489	3.279079
36	1	0	-1.988017	5.068039	-2.316925
37	1	0	1.899764	-1.726469	-3.822829
38	1	0	-2.784999	2.906567	-2.746589
39	1	0	3.038714	5.982874	-5.783664
40	1	0	2.588714	2.366038	4.622393
41	1	0	2.284896	7.428762	-3.928171
42	1	0	3.476659	-0.546537	-4.900355
43	1	0	0.684354	-0.527964	-4.297740
44	1	0	3.854088	5.475912	-2.147393
45	1	0	3.357688	4.607239	1.038322
46	1	0	4.016095	-0.994579	-2.583617
47	1	0	4.408563	6.228127	-3.658419
48	1	0	-2.212495	3.329883	0.869174
49	1	0	2.567938	0.911335	-5.337715
50	1	0	3.503463	4.385746	3.504544
51	1	0	0.720374	6.603871	-3.912974
52	1	0	-1.003564	2.066565	0.669653
53	1	0	4.103953	0.650254	-1.922955
54	1	0	-2.851087	4.847826	-0.791913
55	1	0	3.079547	4.219203	-5.623849
56	1	0	-3.389909	2.440264	-1.144370
57	1	0	0.789149	-1.074203	-2.613400
58	1	0	1.658783	6.759253	-2.413131
59	1	0	1.524846	5.053400	-5.767045
60	1	0	4.464047	4.467800	-3.469208
61	15	0	-1.101517	-0.246685	-0.423046
62	6	0	-0.254285	-0.661885	1.051256
63	6	0	-1.715819	-1.635667	2.833821
64	6	0	-2.277194	-2.792726	3.381923
65	6	0	-0.584693	-1.779404	1.970745
66	6	0	-2.393718	-0.293813	3.231537
67	6	0	-1.816396	-1.603475	-1.401307
68	6	0	-1.746796	-4.064538	3.203589
69	6	0	0.051137	-3.057089	1.878292
70	6	0	-2.354157	-2.730769	-0.766351
71	6	0	-0.553793	-4.154514	2.496607
72	6	0	-3.419850	0.167068	2.179635
73	6	0	-1.917901	-1.469497	-2.789987
74	6	0	1.384904	-3.308063	1.136537
75	6	0	-2.456311	-5.277778	3.808725
76	6	0	2.501150	-2.461682	1.786142
77	6	0	1.870360	-4.765034	1.271700
78	6	0	-1.372514	0.822629	3.496247
79	6	0	-3.034417	-3.603290	-2.915888
80	6	0	-3.177335	-0.447724	4.554707
81	6	0	-2.952030	-3.728313	-1.530554
82	6	0	1.259547	-3.083387	-0.384758
83	6	0	-1.731755	-6.589935	3.492924

84	6	0	-2.521686	-2.470583	-3.543802
85	6	0	-2.529563	-5.121086	5.337002
86	6	0	-3.881415	-5.364517	3.236934
87	1	0	-0.094111	-5.126096	2.397280
88	1	0	-3.171913	-2.704189	3.984803
89	1	0	-2.942409	0.519231	1.264086
90	1	0	0.488934	-3.746510	-0.794769
91	1	0	-2.303091	-2.834955	0.314796
92	1	0	1.199407	-5.472745	0.773521
93	1	0	-4.096241	-1.030349	4.437413
94	1	0	2.209412	-1.431818	1.990319
95	1	0	-1.509645	-0.588489	-3.279079
96	1	0	1.988017	-5.068039	2.316925
97	1	0	-1.899764	1.726469	3.822829
98	1	0	2.784999	-2.906567	2.746589
99	1	0	-3.038714	-5.982874	5.783664
100	1	0	-2.588714	-2.366038	-4.622393
101	1	0	-2.284896	-7.428762	3.928171
102	1	0	-3.476659	0.546537	4.900355
103	1	0	-0.684354	0.527964	4.297740
104	1	0	-3.854088	-5.475912	2.147393
105	1	0	-3.357688	-4.607239	-1.038322
106	1	0	-4.016095	0.994579	2.583617
107	1	0	-4.408563	-6.228127	3.658419
108	1	0	2.212495	-3.329883	-0.869174
109	1	0	-2.567938	-0.911335	5.337715
110	1	0	-3.503463	-4.385746	-3.504544
111	1	0	-0.720374	-6.603871	3.912974
112	1	0	1.003564	-2.066565	-0.669653
113	1	0	-4.103953	-0.650254	1.922955
114	1	0	2.851087	-4.847826	0.791913
115	1	0	-3.079547	-4.219203	5.623849
116	1	0	3.389909	-2.440264	1.144370
117	1	0	-0.789149	1.074203	2.613400
118	1	0	-1.658783	-6.759253	2.413131
119	1	0	-1.524846	-5.053400	5.767045
120	1	0	-4.464047	-4.467800	3.469208

Rotational constants (GHZ):	0.0901920	0.0373632	0.0348203

NBO analysis of 7

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
P	1	1.24647	9.99761	3.69903	0.05689	13.75353
C	2	-0.93213	1.99915	4.91449	0.01850	6.93213
C	3	0.00402	1.99900	3.97869	0.01829	5.99598
C	4	-0.23681	1.99901	4.22619	0.01161	6.23681
C	5	-0.06936	1.99892	4.04901	0.02143	6.06936
C	6	-0.07353	1.99915	4.06237	0.01200	6.07353
C	7	-0.39001	1.99890	4.37053	0.02059	6.39001
C	8	-0.02091	1.99902	4.00233	0.01955	6.02091
C	9	0.00699	1.99899	3.97595	0.01807	5.99301
C	10	-0.21939	1.99905	4.20482	0.01552	6.21939
C	11	-0.24059	1.99900	4.23007	0.01152	6.24059
C	12	-0.67137	1.99938	4.66196	0.01003	6.67137
C	13	-0.22493	1.99904	4.21063	0.01525	6.22493
C	14	-0.07577	1.99914	4.06465	0.01197	6.07577
C	15	-0.07514	1.99914	4.06454	0.01146	6.07514
C	16	-0.66028	1.99939	4.65082	0.01007	6.66028
C	17	-0.68608	1.99943	4.67572	0.01093	6.68608
C	18	-0.67104	1.99939	4.66120	0.01045	6.67104
C	19	-0.23271	1.99912	4.21985	0.01374	6.23271
C	20	-0.68283	1.99943	4.67277	0.01063	6.68283
C	21	-0.23269	1.99912	4.21948	0.01410	6.23269
C	22	-0.66590	1.99939	4.65594	0.01057	6.66590
C	23	-0.68658	1.99942	4.67652	0.01064	6.68658
C	24	-0.23262	1.99911	4.21939	0.01413	6.23262
C	25	-0.67286	1.99941	4.66349	0.00996	6.67286
C	26	-0.67164	1.99941	4.66228	0.00995	6.67164
H	27	0.23842	0.00000	0.76006	0.00152	0.76158
H	28	0.23151	0.00000	0.76731	0.00119	0.76849
H	29	0.23666	0.00000	0.76215	0.00119	0.76334
H	30	0.24045	0.00000	0.75854	0.00101	0.75955
H	31	0.26025	0.00000	0.73822	0.00153	0.73975
H	32	0.23571	0.00000	0.76339	0.00089	0.76429
H	33	0.22889	0.00000	0.77028	0.00082	0.77111
H	34	0.22181	0.00000	0.77717	0.00102	0.77819
H	35	0.25076	0.00000	0.74812	0.00112	0.74924
H	36	0.23491	0.00000	0.76417	0.00092	0.76509
H	37	0.23179	0.00000	0.76729	0.00092	0.76821
H	38	0.23664	0.00000	0.76233	0.00103	0.76336
H	39	0.23295	0.00000	0.76614	0.00091	0.76705
H	40	0.24738	0.00000	0.75188	0.00074	0.75262
H	41	0.24007	0.00000	0.75912	0.00081	0.75993
H	42	0.23960	0.00000	0.75957	0.00083	0.76040
H	43	0.22853	0.00000	0.77054	0.00093	0.77147
H	44	0.23571	0.00000	0.76338	0.00091	0.76429
H	45	0.24643	0.00000	0.75277	0.00080	0.75357
H	46	0.23178	0.00000	0.76721	0.00100	0.76822
H	47	0.23357	0.00000	0.76552	0.00091	0.76643
H	48	0.23205	0.00000	0.76701	0.00094	0.76795
H	49	0.23986	0.00000	0.75927	0.00087	0.76014
H	50	0.24503	0.00000	0.75426	0.00072	0.75497
H	51	0.23686	0.00000	0.76225	0.00088	0.76314

H	52	0.22731	0.00000	0.76971	0.00298	0.77269
H	53	0.23485	0.00000	0.76426	0.00089	0.76515
H	54	0.24222	0.00000	0.75698	0.00081	0.75778
H	55	0.23382	0.00000	0.76548	0.00071	0.76618
H	56	0.23635	0.00000	0.76279	0.00086	0.76365
H	57	0.24377	0.00000	0.75446	0.00177	0.75623
H	58	0.23689	0.00000	0.76219	0.00092	0.76311
H	59	0.24019	0.00000	0.75899	0.00082	0.75981
H	60	0.23468	0.00000	0.76461	0.00071	0.76532
P	61	1.24647	9.99761	3.69903	0.05689	13.75353
C	62	-0.93213	1.99915	4.91449	0.01850	6.93213
C	63	0.00402	1.99900	3.97869	0.01829	5.99598
C	64	-0.23681	1.99901	4.22619	0.01161	6.23681
C	65	-0.06936	1.99892	4.04901	0.02143	6.06936
C	66	-0.07353	1.99915	4.06237	0.01200	6.07353
C	67	-0.39001	1.99890	4.37053	0.02059	6.39001
C	68	-0.02091	1.99902	4.00233	0.01955	6.02091
C	69	0.00699	1.99899	3.97595	0.01807	5.99301
C	70	-0.21939	1.99905	4.20482	0.01552	6.21939
C	71	-0.24059	1.99900	4.23007	0.01152	6.24059
C	72	-0.67137	1.99938	4.66196	0.01003	6.67137
C	73	-0.22493	1.99904	4.21063	0.01525	6.22493
C	74	-0.07577	1.99914	4.06465	0.01197	6.07577
C	75	-0.07514	1.99914	4.06454	0.01146	6.07514
C	76	-0.66028	1.99939	4.65082	0.01007	6.66028
C	77	-0.68608	1.99943	4.67572	0.01093	6.68608
C	78	-0.67104	1.99939	4.66120	0.01045	6.67104
C	79	-0.23271	1.99912	4.21985	0.01374	6.23271
C	80	-0.68283	1.99943	4.67277	0.01063	6.68283
C	81	-0.23269	1.99912	4.21948	0.01410	6.23269
C	82	-0.66590	1.99939	4.65594	0.01057	6.66590
C	83	-0.68658	1.99942	4.67652	0.01064	6.68658
C	84	-0.23262	1.99911	4.21939	0.01413	6.23262
C	85	-0.67286	1.99941	4.66349	0.00996	6.67286
C	86	-0.67164	1.99941	4.66228	0.00995	6.67164
H	87	0.23842	0.00000	0.76006	0.00152	0.76158
H	88	0.23151	0.00000	0.76731	0.00119	0.76849
H	89	0.23666	0.00000	0.76215	0.00119	0.76334
H	90	0.24045	0.00000	0.75854	0.00101	0.75955
H	91	0.26025	0.00000	0.73822	0.00153	0.73975
H	92	0.23571	0.00000	0.76339	0.00089	0.76429
H	93	0.22889	0.00000	0.77028	0.00082	0.77111
H	94	0.22181	0.00000	0.77717	0.00102	0.77819
H	95	0.25076	0.00000	0.74812	0.00112	0.74924
H	96	0.23491	0.00000	0.76417	0.00092	0.76509
H	97	0.23179	0.00000	0.76729	0.00092	0.76821
H	98	0.23664	0.00000	0.76233	0.00103	0.76336
H	99	0.23295	0.00000	0.76614	0.00091	0.76705
H	100	0.24738	0.00000	0.75188	0.00074	0.75262
H	101	0.24007	0.00000	0.75912	0.00081	0.75993
H	102	0.23960	0.00000	0.75957	0.00083	0.76040
H	103	0.22853	0.00000	0.77054	0.00093	0.77147
H	104	0.23571	0.00000	0.76338	0.00091	0.76429
H	105	0.24643	0.00000	0.75277	0.00080	0.75357
H	106	0.23178	0.00000	0.76721	0.00100	0.76822
H	107	0.23357	0.00000	0.76552	0.00091	0.76643
H	108	0.23205	0.00000	0.76701	0.00094	0.76795
H	109	0.23986	0.00000	0.75927	0.00087	0.76014

H	110	0.24503	0.00000	0.75426	0.00072	0.75497
H	111	0.23686	0.00000	0.76225	0.00088	0.76314
H	112	0.22731	0.00000	0.76971	0.00298	0.77269
H	113	0.23485	0.00000	0.76426	0.00089	0.76515
H	114	0.24222	0.00000	0.75698	0.00081	0.75778
H	115	0.23382	0.00000	0.76548	0.00071	0.76618
H	116	0.23635	0.00000	0.76279	0.00086	0.76365
H	117	0.24377	0.00000	0.75446	0.00177	0.75623
H	118	0.23689	0.00000	0.76219	0.00092	0.76311
H	119	0.24019	0.00000	0.75899	0.00082	0.75981
H	120	0.23468	0.00000	0.76461	0.00071	0.76532
* Total *		0.00000	119.95426	277.18031	0.86543	398.00000

Natural Population

Core	119.95426 (99.9619% of 120)
Valence	277.18031 (99.7051% of 278)
Natural Minimal Basis	397.13457 (99.7826% of 398)
Natural Rydberg Basis	0.86543 (0.2174% of 398)

UV-Vis absorption properties of 7

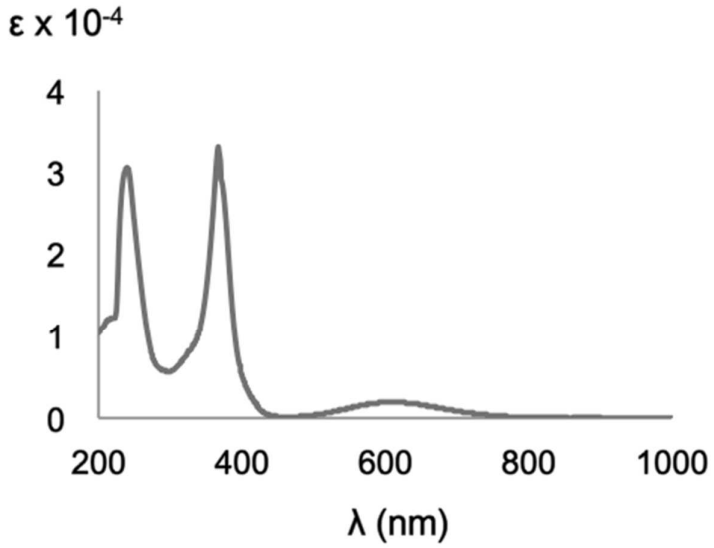


Figure S7. UV-Vis spectra of **7** in dichloromethane.

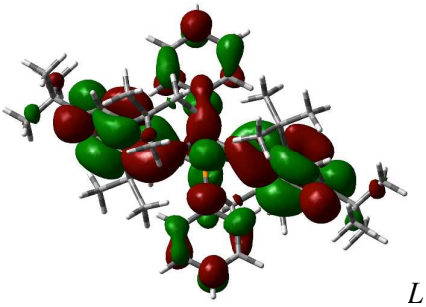
TD-SCF calculation of 7

#p td=(nstates=10) m062x/6-31g(d) guess=mix

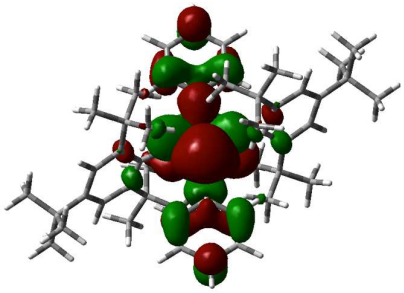
Excited State 1: Singlet-AU 2.2307 eV 555.80 nm f=0.0527 <S**2>=0.000
199 ->200 0.69240
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2627.84715549
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-AU 3.5809 eV 346.24 nm f=0.4005 <S**2>=0.000
198 ->200 0.69611

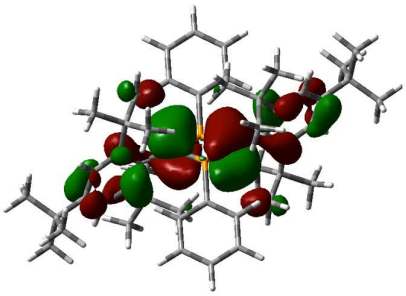
Excited State 4: Singlet-AU 3.7231 eV 333.01 nm f=0.1133 <S**2>=0.000
199 ->201 0.67291



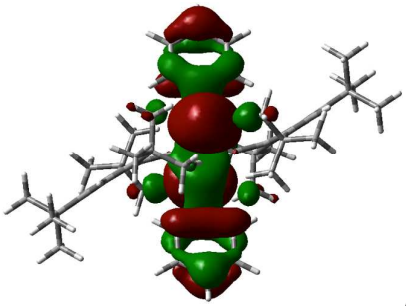
LUMO+1 (#201): +0.41 eV



LUMO (#200): –1.12 eV



HOMO (#199): –5.72 eV



HOMO–1 (#198): –6.61 eV

Figure S8. Selected molecular orbitals of **7**.

Redox properties of 7

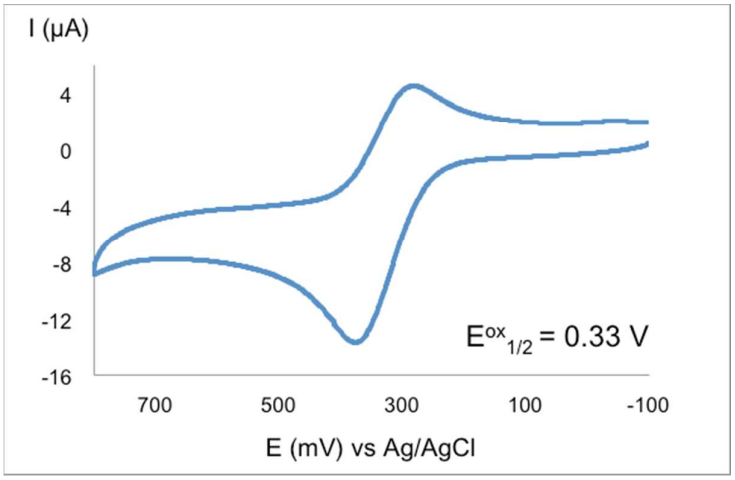


Figure S9. Cyclic voltammograms of **7**. *Conditions*: 1 mM in CH_2Cl_2, 0.1 M TBAP, working: GC, counter: Pt, reference: Ag/AgCl, 20 °C; scan rate: 50 mVs^{-1}.

X-ray Electron Density Distribution Analysis of 7

Diffraction data collection of 7

A prism shaped and blue single crystal of **7** 0.23 × 0.20 × 0.13 mm, was selected for measurements. The diffraction data were collected using a RIGAKU AFC-8 diffractometer equipped with a Saturn70 CCD detector with Mo*K*α radiation by an oscillation method at 90 K. X-rays were monochromated and focused by a confocal mirror. Twelve data sets were measured with different crystal orientations and detector positions; (i) $\chi = 50°$, $\phi = 0°$ and $2\theta = 20°$ and (ii) $\chi = 50°$, $\phi = 90°$ and $2\theta = 20°$, (iii) $\chi = 50°$, $\phi = 0°$ and $2\theta = 40°$, (iv) $\chi = 50°$, $\phi = 90°$ and $2\theta = 40°$, (v) $\chi = 0°$, $\phi = 180°$ and $2\theta = 40°$, (vi) $\chi = 50°$, $\phi = 270°$ and $2\theta = 40°$, (vii) $\chi = 0°$, $\phi = 0°$ and $2\theta = 40°$, (viii) $\chi = 50°$, $\phi = 0$ and $2\theta = 83°$, (ix) $\chi = 50°$, $\phi = 90°$ and $2\theta = 83°$, (x) $\chi = 0°$, $\phi = 180°$ and $2\theta = 83°$, (xi) $\chi = 50°$, $\phi = 270°$ and $2\theta = 83°$, and (xii) $\chi = 0°$, $\phi = 0°$ and $2\theta = 83°$. Exposure time and oscillation angle for each frame were 0.3 sec and 0.3°, 2 sec and 0.5°, and 16 sec and 0.5° for the data sets with 2θ = 20, 40 and 83°, respectively. For all data sets, camera distance was set at 40 mm. Bragg spots were integrated, scaled and averaged up to $\sin\theta/\lambda = 1.22$ Å^{-1} by the program HKL2000.[S8] Lorentz and polarization corrections were applied during the scaling processes. No absorption corrections were applied.

The number of measured and independent reflections, completeness, and R_{int} were 126954, 32088, 0.966 and 0.0364, respectively, up to $\sin\theta/\lambda = 1.22$ Å^{-1}.

Crystal structure and electron density analysis of 7

The initial structure of **7** was solved by a direct method using the programs SIR2004,[S9] and refined by a full matrix least-squares method using the program SHELXL97.[S10] All hydrogen atoms were located on difference Fourier maps, and refined their positions and isotropic temperature factors. High order refinements were carried out in order to determine the position of non-hydrogen atoms using 28117 independent reflections with $\sin\theta/\lambda \geq 0.625$ Å^{-1}. On the refinements, the positions of the hydrogen atoms bonding to carbon atoms were constrained to be C–H distances of 1.083 and 1.059 Å for the aromatic and methyl groups, respectively.

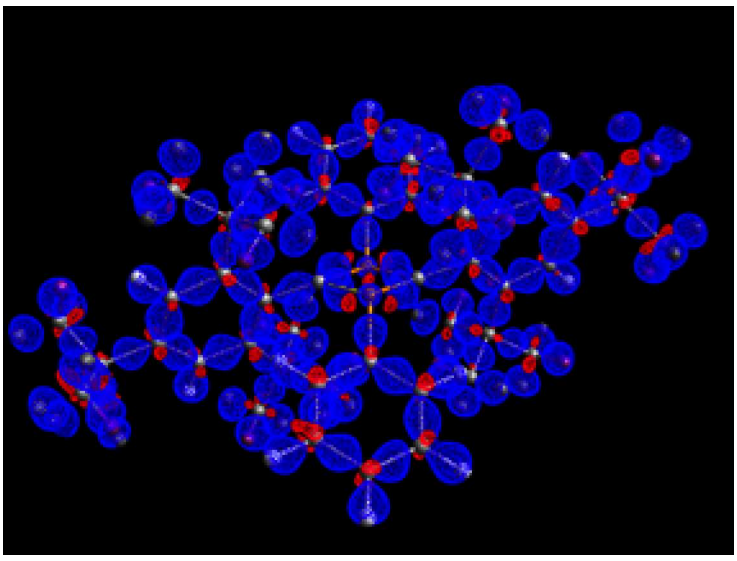
Refinements of a multipole expansion method using the Hansen-Coppens multipole formalism[S11] and topologaical analyses based on resulted parameters were performed with the XD2006 package.[S12] The refinements were carried out against 28117 independent reflections of $\sin\theta/\lambda \leq 1.22$ Å^{-1} with $I > 3\sigma(I)$ based on F^2. At the first stage of the

refinements, the atomic coordinates and temperature factors of the atoms were fixed on those of the high order refinement. The population parameters, P_v, $P_{lm\pm}$ of the non-hydrogen atoms and scale were refined. The levels of the multipoles were raised up stepwise to hexadecapole and octupole for P1 and C1, and other C atoms, respectively, and dipole along bond for H atoms. Chemical equivalent constraints were applied for multipole parameters of all atoms. The radial screening parameters, κ and κ' were refined after refinements of multipole parameters at hexadecapole level for non-hydrogen atoms. The refinement cycles were repeated twice. At the second stage, the temperature factors were refined by applying harmonic anisotropic models for non-H atoms, following the refinements of the radial screening parameters, κ and κ'. The chemical equivalent constraints on the multipole parameters were relaxed gradually, and finally only the hydrogen atoms were constrained. The stage was repeated to make the shifts of the parameters converged. At the final stage, the coordinates, multipoles, temperature factors were refined. The C−H distances were constrained to be 1.083 and 1.059 Å for the aromatic and methyl groups, respectively. The number of parameters in the final cycle of the refinements was 780. The number of electrons in the crystal was constrained.

Crystal data: $C_{50}H_{68}P_2$, FW = 730.98, monoclinic, space group P-1, a = 8.6852(1) Å, b = 11.6707(2) Å, c = 11.6814(1) Å, α = 67.5380(7)°, β = 89.0645(7)°, γ = 84.0390(1)°, V = 1087.96(2) Å^3; D_X = 1.116 Mg m^{-3}; Z = 1; μ(Mo $K\alpha$) = 0.132 mm^{-1}. $R(F)$ = 0.0213, $wR(F^2)$ = 0.0399, and S = 1.09 for 22245 reflections of $(\sin\theta / \lambda)_{max}$ = 1.22 Å^{-1} with $I > 3\sigma(I)$. $\Delta\rho_{min}$, $_{max}$ = −0.30, 0.24 e Å^{-3}

(CCDC-957260/957261)

(a)



(b)

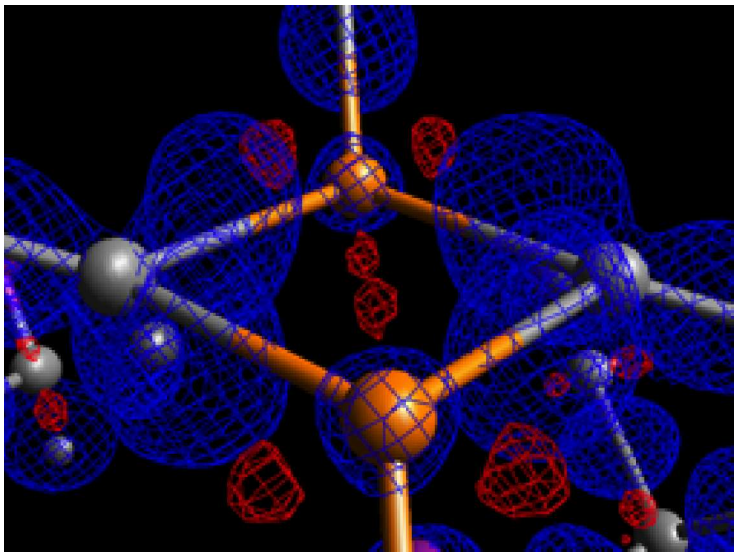


Figure S10. Electron density maps of **7**. (a) 3D view plot displaying electron-increased (blue) and electron-decreased (red) areas by construction of the molecule. (b) A magnification plot of the electron-density map around the PCPC ring.

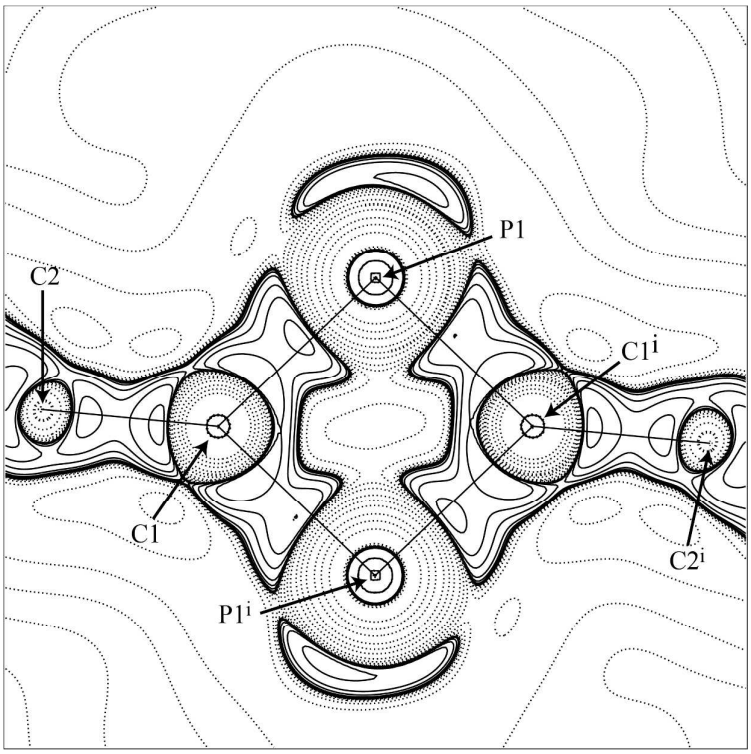


Figure S11. Laplacian [$\nabla^2(\rho)$] distribution plot of **7** on the PCPC plane. Solid and dotted lines indicate negative and positive $\nabla^2(\rho)$ value, respectively. The contours are drawn at $\pm 2 \times 10^n$, $\pm 4 \times 10^n$ and $\pm 8 \times 10^n$ (where $n = -2, -1, 0, 1, 2$) e Å^{-5}.

AIM Analysis of 7

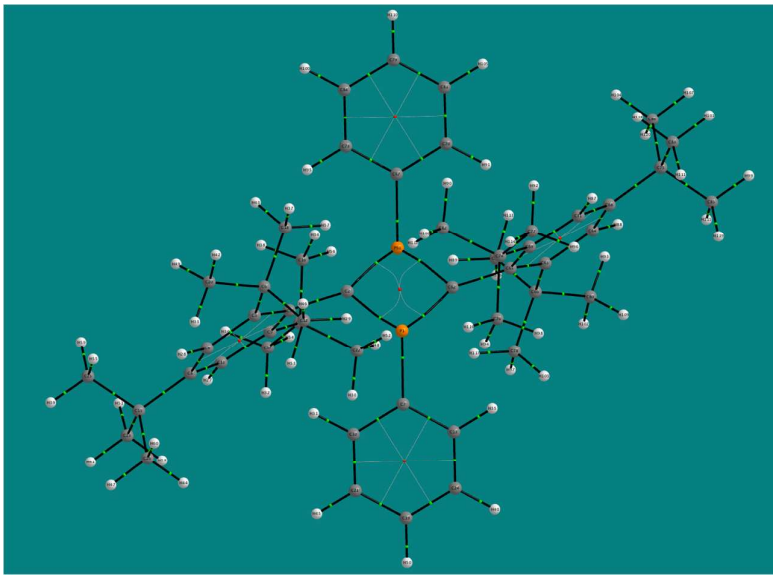


Figure S12. Selected BCP (green) and RCP (red) for **7** [HF/6-31G(d)//M06-2X/6-31G(d)].

X-ray Electron Density Distribution Analysis of B

Diffraction data collection of B

A prism shaped and blue single crystal of **B**, 0.13 × 0.09 × 0.06 mm, was selected for measurements. The diffraction data were collected using a RIGAKU AFC-8 diffractometer equipped with a Saturn70 CCD detector with Mo$K\alpha$ radiation by an oscillation method at 90 K. X-rays were monochromated and focused by a confocal mirror. Twelve data sets were measured with different crystal orientations and detector positions; (i) $\chi = 50°$, $\phi = 90°$ and $2\theta = 20°$, (ii) $\chi = 0°$, $\phi = 0°$ and $2\theta = 20°$, (iii) $\chi = 50°$, $\phi = 0°$ and $2\theta = 40°$, (iv) $\chi = 50°$, $\phi = 90°$ and $2\theta = 40°$, (v) $\chi = 50°$, $\phi = 180°$ and $2\theta = 40°$, (vi) $\chi = 50°$, $\phi = 270°$ and $2\theta = 40°$, (vii) $\chi = 0°$, $\phi = 0°$ and $2\theta = 40°$, (viii) $\chi = 50°$, $\phi = 0°$ and $2\theta = 83°$, (ix) $\chi = 50°$, $\phi = 90°$ and $2\theta = 83°$, (x) $\chi = 50°$, $\phi = 180°$ and $2\theta = 83°$, (xi) $\chi = 50°$, $\phi = 270°$ and $2\theta = 83°$, and (xii) $\chi = 0°$, $\phi = 0°$ and $2\theta = 83°$. Exposure time and oscillation angle for each frame were 5 sec and 0.5°, 32 sec and 0.5°, and 128 sec and 0.5° for the data sets with 2θ = 20, 40 and 83°, respectively. For all data sets, camera distance was set at 40 mm, respectively. Bragg spots were integrated, scaled and averaged up to $\sin\theta/\lambda = 1.00$ Å^{-1} by the program HKL2000.[S10] Lorentz and polarization corrections were applied during the scaling processes. Analytical absorption corrections based on the specimen shape[S13] were applied.

The number of measured and independent reflections, completeness, and R_{int} were 294615, 36568, 0.992 and 0.0496, respectively, up to $\sin\theta/\lambda = 1.00$ Å^{-1}.

Crystal structure and electron density analysis of B

The initial structure of **B** was solved by a direct method using the programs SIR2004,[S9] and refined by a full matrix least-squares method on F^2 using the program SHELXL97.[S10] All hydrogen atoms were located on difference Fourier maps. The hydrogen atoms of the methyl groups were refined as riding models, and others were refined isotropically. High order refinements were carried out in order to determine the position of non-hydrogen atoms using 28515 independent reflections with $\sin\theta/\lambda \geq 0.625$ Å^{-1}. On the refinements, the positions of the hydrogen atoms bonding to carbon atoms were constrained to be C–H distances of 1.083, 1.059 and 1.092 Å for the aromatic, methyl, methylene, and methyne groups, respectively.

Refinements of a multipole expansion method using the Hansen-Coppens multipole formalism[S11] and topologaical analyses based on resulted parameters were performed with the XD2006 package.[S12] The refinements were carried out against 30524 independent reflections of $\sin\theta/\lambda \leq 1.00$ Å^{-1} with $I > 3\sigma(I)$ based on F^2. At the first stage of the refinements, the atomic coordinates and temperature factors of the atoms were fixed on those

of the high order refinement. The population parameters, P_v, $P_{lm\pm}$ of the non-hydrogen atoms and scale were refined. The levels of the multipoles were raised up stepwise to hexadecapole and octupole for P1, P2, C1 and C2 and other C atoms, respectively, and dipole along bond for H atoms. Chemical equivalent constraints were applied for multipole parameters of all atoms. The radial screening parameters, κ and κ' were refined after refinements of multipole parameters at hexadecapole level for non-hydrogen atoms. The refinement cycles were repeated twice. At the second stage, the temperature factors were refined by applying harmonic anisotropic models for non-H atoms, 4th-order anharmonic anisotropic models for C47A, C48A and C49A atoms in *t*-butyl group on P2, and isotropic models for H atoms, following the refinements of the radial screening parameters, κ and κ'. The chemical equivalent constraints on the multipole parameters were relaxed gradually, and finally only the hydrogen atoms were constrained. The stage was repeated to make the shifts of the parameters converged. At the final stage, the coordinates, multipoles, temperature factors were refined. The C−H distances were constrained to be 1.083, 1.059 and 1.092 Å for the aromatic, methyl, methylene, and methyne groups, respectively. The number of parameters in the final cycle of the refinements was 1516. The number of electrons in the crystal was constrained.

Crystal data: $C_{49}H_{74}P_2$, FW = 725.02, monoclinic, space group $P2_1/c$, a = 17.4396(3) Å, b = 23.2554(3) Å, c = 10.9080(1) Å, β = 95.4413(9)°, V = 4403.97(10) Å^3; D_X = 1.093 Mg m^{-3}; Z = 4; μ(Mo $K\alpha$) = 0.130 mm^{-1}. $R(F)$ = 0.0224, $wR(F^2)$ = 0.0283, and S = 0.78 for 24697 reflections of $(\sin\theta/\lambda)_{max}$ = 1.00 Å^{-1} with $I > 3\sigma(I)$. $\Delta\rho_{min,\ max}$ = −0.22, 0.27 e Å^{-3}

(CCDC-957262/957263)

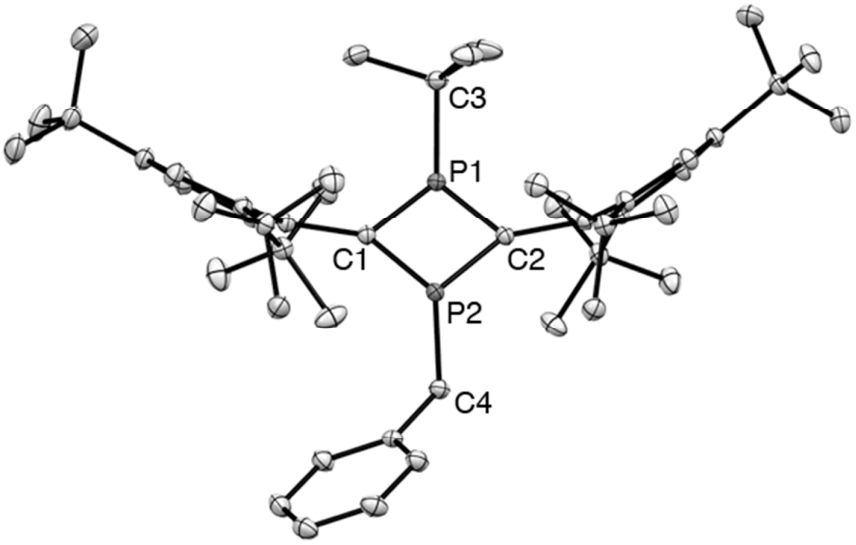


Figure S13. X-ray structure of **B** in a non-solvate crystal determined by the data listed in Table S2. Hydrogen atoms are omitted for clarity. The *t*-butyl group at the P1 atom is disordered and the atoms with predominant occupancy factor (0.72) are shown. Angles between the C_2P_2 four-membered ring and two Mes* aromatic rings are 61.52° (C1 side) and 64.29° (C2 side), respectively. Selected bond lengths (Å) and angles (°): P1–C1 1.7261(4), P2–C1 1.7950(5), P1–C2 1.7238(5), P2–C2 1.7868(4), P1–C3 1.8695(5), P2–C4 1.8694(5), C1–Mes* 1.4862(7), C2–Mes* 1.4828(7), C1–P1–C2 94.15(2), C1–P2–C2 89.71(2), P1–C1–P2 87.83(2), P1–C2–P2 88.17(2); Σ_{angles}C1 359.56, Σ_{angles}C2 359.08, Σ_{angles}P1 342.03, Σ_{angles}P2 321.34.

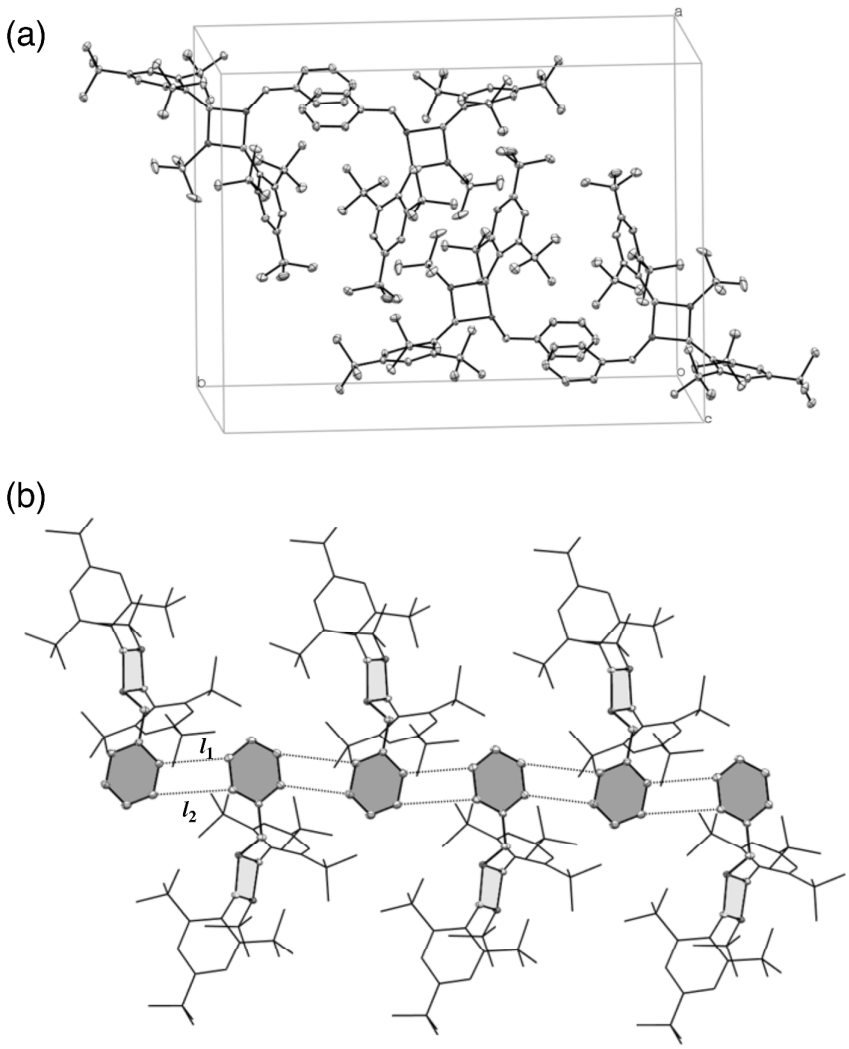


Figure S14. (a) Crystal structure of **B** in the unit cell. (b) Edge-stacking of the benzyl groups along the *c* axis. The benzyl aromatic rings and biradical skeletons are displayed with gray and light gray, respectively. The edge contacts are indicated by dashed lines. The edge-to-edge distances: l_1 = 3.4349(7), l_2 = 3.8293(8) Å.

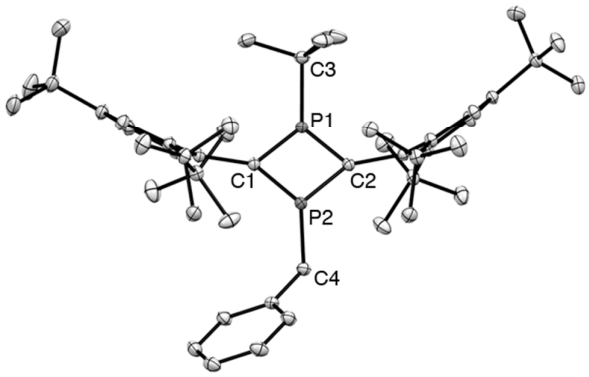


Table S2. Metric Parameters of **B** (distance: Å, angles: °)

	B (X-ray)	**B**·3$CHCl_3$ (X-ray) [a]	**B** (DFT) [b]
P1–C1	1.7261(4)	1.718(5)	1.711
P2–C1	1.7950(5)	1.811(5)	1.808
P1–C2	1.7238(5)	1.713(5)	1.712
P2–C2	1.7868(4)	1.797(5)	1.805
P1–C3	1.8695(5)	1.866(6)	1.873
P2–C4	1.8694(5)	1.893(6)	1.879
C1–C_{Mes*}	1.4862(7)	1.481(7)	1.482
C2–C_{Mes*}	1.4828(7)	1.488(7)	1.479
C1–P1–C2	94.15(2)	95.1(2)	95.31
C1–P2–C2	89.71(2)	89.1(2)	88.89
P1–C1–P2	87.83(2)	87.5(2)	87.72
P1–C2–P2	88.17(2)	88.1(2)	87.76
Σ_{angles}C1	359.56	357.2	359.3
Σ_{angles}C2	359.08	360.2	358.4
Σ_{angles}P1	342.03	344.2	344.2
Σ_{angles}P2	321.34	317.9	313.6

[a] Ref. S2. [b] M06-2X/6-31G(d) level.

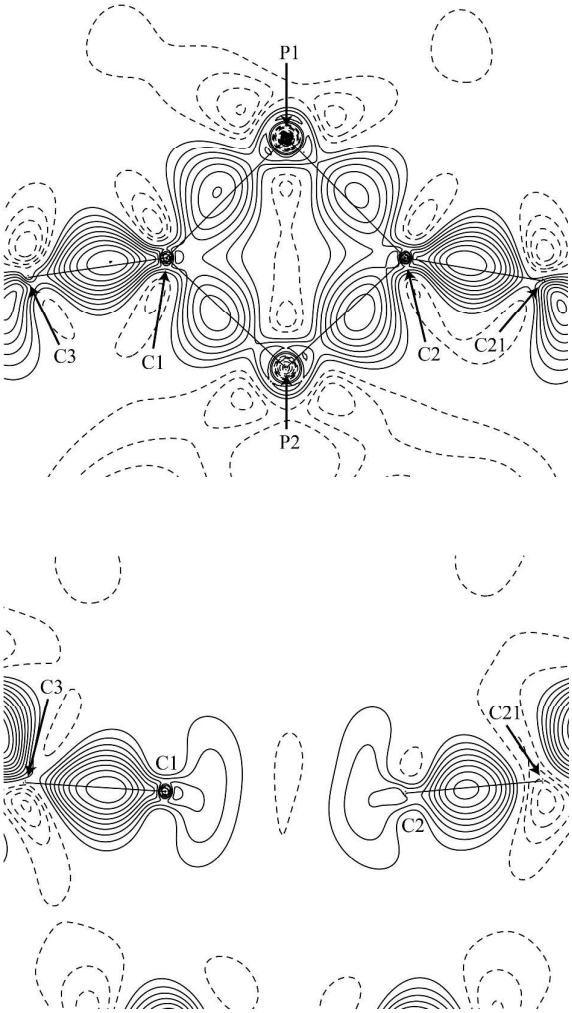


Figure S15. Static model maps of **B** on the PCPC plane (Top) and the cross section of the PCPC plane through the skeletal carbons (bottom). Solid and broken lines indicate positive and negative densities, respectively. The contours are drawn at 0.05 e $Å^{-3}$ interval.

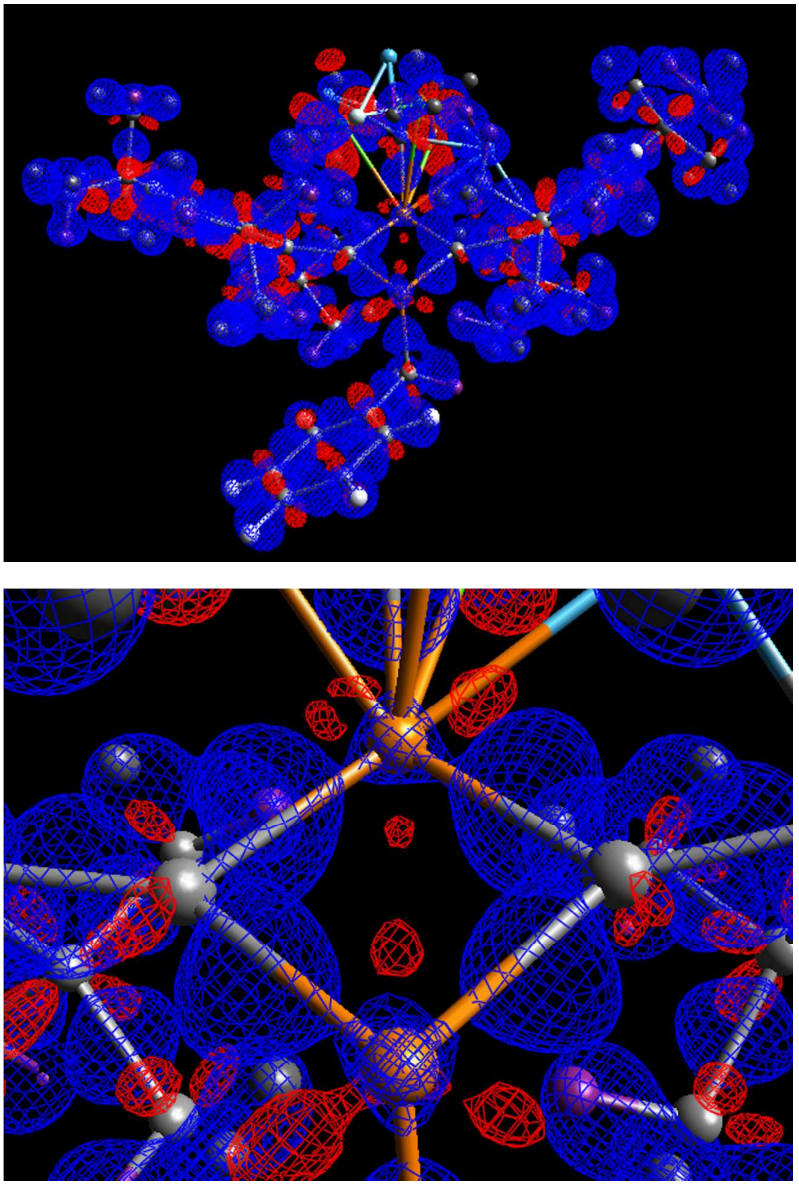


Figure S16. (Top) 3D view plot of **B** displaying electron-increased (blue) and electron-decreased (red) areas by construction of the molecule. (Bottom) A magnification plot of the electron-density map around the PCPC ring.

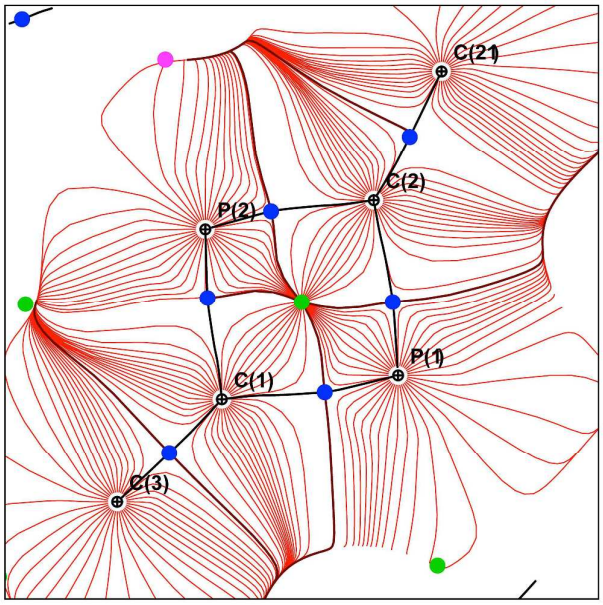


Figure S17. BCP (blue dot) and RCP (green dot) around the 4-membered heterocycle of **B**.

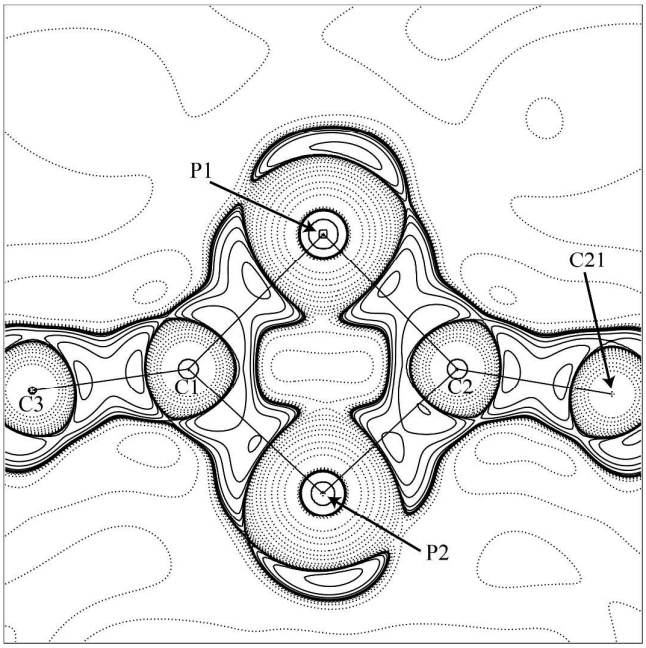
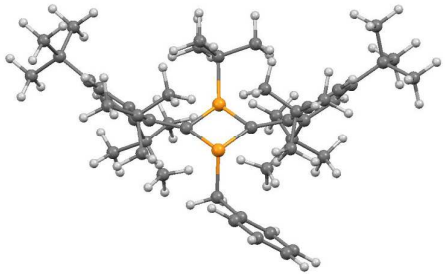


Figure S18. Laplacian [$\nabla^2(\rho)$] distribution plot of **B** on the PCPC plane. Solid and dotted lines indicate negative and positive $\nabla^2(\rho)$ value, respectively. The contours are drawn at $\pm 2 \times 10^n$, $\pm 4 \times 10^n$ and $\pm 8 \times 10^n$ (where $n = -2, -1, 0, 1, 2$) e Å^{-5}.

DFT calculations for B

DFT calculations were carried out with Gaussian 09 program package.[S3] The structures were optimize by use of the M06-2X Hamiltonian accounting for the "medium-range" correlations[S4,S5] and the 6-31G(d) basis sets. AIM[S6] calculations were performed with AIMAll software package.[S7]

DFT optimized structure of B



#p opt m062x/6–31g(d) guess=mix

Stoichiometry	C49H74P2			
Framework group	C1[X(C49H74P2)]			
Deg. of freedom	369			
Full point group		C1	NOp	1
Largest Abelian subgroup		C1	NOp	1
Largest concise Abelian subgroup		C1	NOp	1

E(RM062X) = –2593.44424302 A.U.
Dipole moment (field–independent basis, Debye):
X= –0.0411 Y= –1.2640 Z= –0.2326 Tot= 1.2859

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.010509	1.638010	0.034989
2	15	0	–0.280035	–0.776744	0.214340
3	6	0	–1.393653	0.523000	0.237964
4	6	0	1.115402	0.211431	0.150220
5	6	0	–3.533248	–0.331105	1.169034
6	6	0	–4.857030	0.161319	–1.226185
7	6	0	0.129479	2.820715	1.490074
8	6	0	4.384860	–0.913270	–1.375915
9	6	0	–3.161706	1.862413	–2.002491
10	6	0	2.980769	0.991442	–2.225960
11	6	0	1.200938	3.854145	1.263055
12	6	0	–5.389801	–0.796165	–0.364773
13	6	0	–6.661551	–1.588430	–0.670261
14	6	0	–4.732484	–0.973769	0.846777
15	6	0	2.519296	–0.247033	0.032131
16	6	0	4.098591	–1.958901	0.726197
17	6	0	–0.524674	–2.348322	–0.774932
18	6	0	2.931607	2.377854	–1.554956
19	6	0	–2.864832	0.403120	0.142684
20	6	0	3.299038	–0.075041	–1.161539

21	6	0	1.067124	4.797578	0.238102
22	6	0	4.764992	–1.921519	–0.484227
23	6	0	–2.001345	1.364815	–2.879949
24	6	0	2.561111	–1.173761	2.522822
25	6	0	–3.626120	0.782551	–1.005546
26	6	0	2.075475	5.719752	–0.014998
27	6	0	–7.728232	–1.302329	0.399894
28	6	0	4.070385	1.098266	–3.307627
29	6	0	–2.248209	0.810490	3.085536
30	6	0	2.364784	3.864292	2.033544
31	6	0	–4.362619	–0.342241	3.549851
32	6	0	–2.800789	3.141061	–1.220120
33	6	0	3.034771	–1.097225	1.046319
34	6	0	–3.098119	–0.396122	2.658825
35	6	0	1.683225	0.639747	–2.975893
36	6	0	1.763789	–2.463024	2.777671
37	6	0	–7.247950	–1.234374	–2.040519
38	6	0	–2.350683	–1.691522	3.009414
39	6	0	–4.278470	2.282849	–2.974007
40	6	0	3.378575	4.785829	1.780609
41	6	0	7.187294	–2.099121	–1.108272
42	1	0	7.999381	–2.782861	–1.381306
43	1	0	7.485773	–1.550566	–0.208894
44	1	0	7.070167	–1.375279	–1.920728
45	6	0	3.238909	5.713735	0.753788
46	6	0	3.809710	–1.191731	3.438562
47	6	0	1.739652	0.032851	3.002977
48	6	0	5.890510	–2.886666	–0.857832
49	6	0	–6.321276	–3.088532	–0.662820
50	6	0	0.854012	–2.969632	–1.029789
51	6	0	6.158637	–3.915847	0.244218
52	6	0	5.497842	–3.641423	–2.139277
53	6	0	–1.416200	–3.308682	0.021798
54	6	0	–1.211354	–1.992497	–2.098475
55	1	0	–0.860558	3.291297	1.546895
56	1	0	–7.548640	–0.182310	–2.090520
57	1	0	4.406502	–2.686634	1.466130
58	1	0	–5.408481	0.411695	–2.121783
59	1	0	4.430083	–0.307481	3.258338
60	1	0	1.745679	0.057293	4.098723
61	1	0	3.825429	1.941341	–3.962437
62	1	0	4.028354	6.431892	0.554979
63	1	0	–2.308448	3.866671	–1.878157
64	1	0	–1.244510	0.769363	2.671305
65	1	0	2.475695	3.147577	2.842812
66	1	0	–2.165309	0.825868	4.177955
67	1	0	–3.924899	3.132511	–3.568166
68	1	0	–5.558983	–3.313853	–1.416639
69	1	0	4.948829	–0.810828	–2.294898
70	1	0	–4.542734	1.483875	–3.674204
71	1	0	–2.180245	–1.745404	4.091598
72	1	0	–7.382360	–1.581084	1.400277
73	1	0	5.058009	1.287010	–2.874231
74	1	0	2.457729	3.114308	–2.214369
75	1	0	4.126843	0.201664	–3.933905
76	1	0	1.955303	6.445239	–0.813968
77	1	0	–2.928869	–2.573932	2.711603
78	1	0	–5.183660	2.596769	–2.443794

79	1	0	–1.155217	1.014757	–2.294296
80	1	0	0.166214	4.794524	–0.372712
81	1	0	–5.184655	–1.628265	1.584822
82	1	0	–5.934989	–3.406219	0.310953
83	1	0	0.290926	2.277605	2.423444
84	1	0	–2.711489	1.750560	2.763006
85	1	0	–4.059746	–0.214109	4.594111
86	1	0	–3.713839	3.599689	–0.824254
87	1	0	4.434772	–2.076554	3.303786
88	1	0	1.479643	–2.535576	3.834580
89	1	0	–2.344401	0.538973	–3.513896
90	1	0	3.950199	2.719420	–1.337776
91	1	0	–8.137659	–1.844262	–2.229570
92	1	0	–1.649855	2.172618	–3.533171
93	1	0	0.836993	0.513003	–2.305375
94	1	0	6.955776	–4.595895	–0.073930
95	1	0	2.176854	0.965493	2.632749
96	1	0	0.700208	–0.007945	2.680882
97	1	0	–1.375138	–1.735543	2.515747
98	1	0	–2.144761	2.951431	–0.370683
99	1	0	6.481009	–3.434788	1.174103
100	1	0	–4.957591	–1.257913	3.503201
101	1	0	6.288025	–4.345386	–2.424845
102	1	0	4.277797	4.777190	2.389083
103	1	0	1.433369	1.429376	–3.694630
104	1	0	–6.531081	–1.426741	–2.846009
105	1	0	–7.213718	–3.685030	–0.884679
106	1	0	–7.982773	–0.237515	0.416125
107	1	0	3.490741	–1.180482	4.485959
108	1	0	0.843644	–2.479166	2.182667
109	1	0	5.339038	–2.954398	–2.976487
110	1	0	–8.640796	–1.871710	0.188749
111	1	0	2.395572	2.381910	–0.607416
112	1	0	5.268634	–4.517722	0.457738
113	1	0	2.350262	–3.351964	2.519126
114	1	0	1.822711	–0.295796	–3.531862
115	1	0	4.571159	–4.205153	–1.986010
116	1	0	–5.005303	0.499218	3.271914
117	1	0	–1.374216	–2.917777	–2.666842
118	1	0	–0.592315	–1.324467	–2.704864
119	1	0	–2.182963	–1.514157	–1.931731
120	1	0	0.713304	–3.897099	–1.598924
121	1	0	1.375994	–3.217459	–0.099456
122	1	0	1.499949	–2.301471	–1.609397
123	1	0	–1.574902	–4.216369	–0.573640
124	1	0	–0.955462	–3.603709	0.970437
125	1	0	–2.395666	–2.864092	0.232509

Rotational constants (GHZ): 0.0773697 0.0402163 0.0354192

AIM Analysis of B

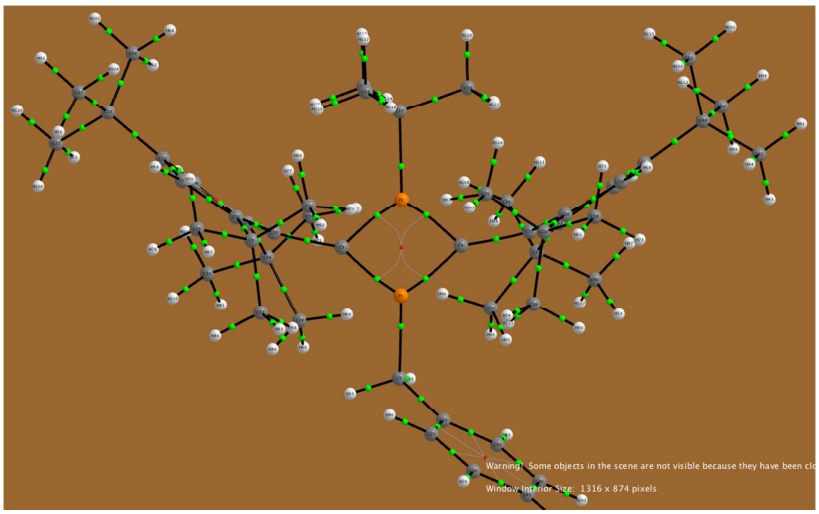


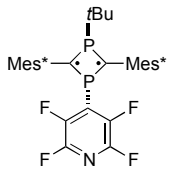
Figure S19. Selected BCP (green) and RCP (red) for **B** [HF/6-31G(d)//M06-2X/6-31G(d)].

Table S3. Conventional Crystal Structure Analysis using X-Ray Diffraction Data for Electron Density Analysis of **7** and **B**

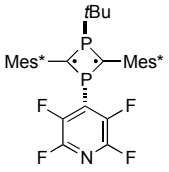
Compound	**7**	**B**
Formula	$C_{50}H_{68}P_2$	$C_{49}H_{74}P_2$
Fw / g mol^{-1}	730.98	725.02
Crystal system	triclinic	monoclinic
Crystal size	0.23 x 0.20 x 0.13 mm^3	0.13 x 0.09 x 0.06 mm^3
Space group	*P*–1 (#2)	$P2_1/c$ (#14)
a / Å	8.6852(1)	17.4396(3)
b / Å	11.6707(2)	23.2554(3)
c / Å	11.6814(1)	10.9080(1)
α / °	67.5380(7)	90
β / °	89.0645(7)	95.4413(9)
γ / °	84.0390(1)	90
V / Å^3	1087.96(2)	4403.97(10)
Z	1	4
T / K	90	90
ρ_{calc} / mg cm^{-3}	1.116	1.093
μ / mm^{-1}	0.132	0.130
□$_{000}$	398	1592
θ_{min} / °	1.89	1.46
θ_{max} / °	60.22	45.29
Observed reflections	126954	297358
Unique reflections	32088	36568
Index ranges	–21≤*h*≤21	–34≤*h*≤34
	–28≤*k*≤28	–46≤*k*≤46
	–28≤*l*≤28	–21≤*l*≤19
Max diffraction density / e Å^{-3}	0.568	0.542
Min diffraction density / e Å^{-3}	–0.478	–0.733
R_{int}	0.0364	0.0496
*R*1 ($I > 2\sigma(I)$)[a]	0.0338	0.0324
w*R*2 (all data)[b]	0.1131	0.0918
Refined parameters	371	504
GOF	1.027	0.917

[a] $R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo|$, [b] $wR2 = [\Sigma \, \{w(Fo^2 - Fc^2)^2 / \, \Sigma \, w(Fo^2)^2\}]^{1/2}$

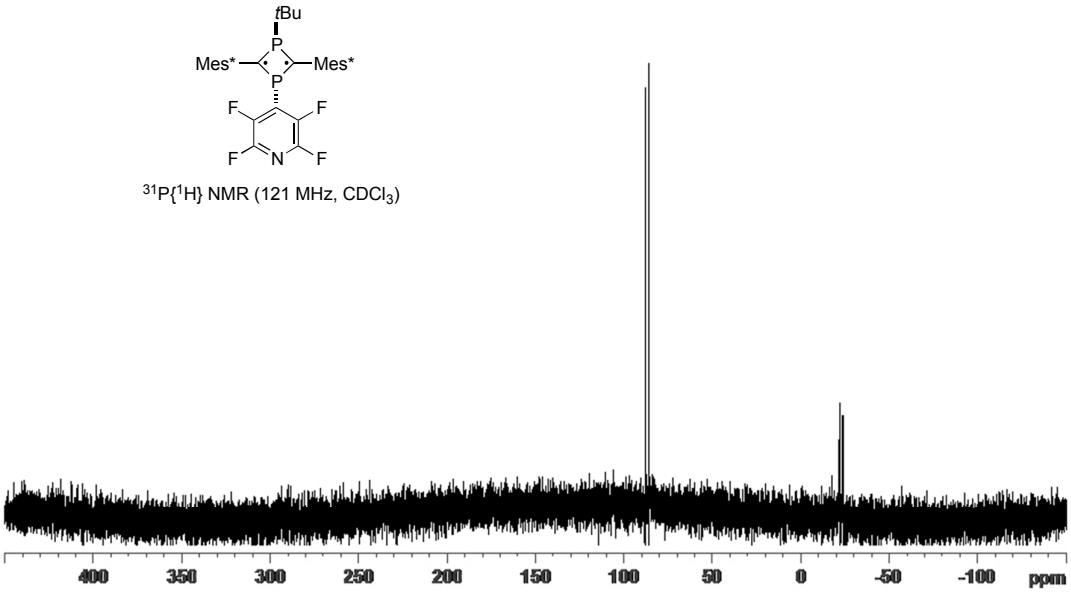
3



^{1}H NMR (300 MHz, $CDCl_3$)

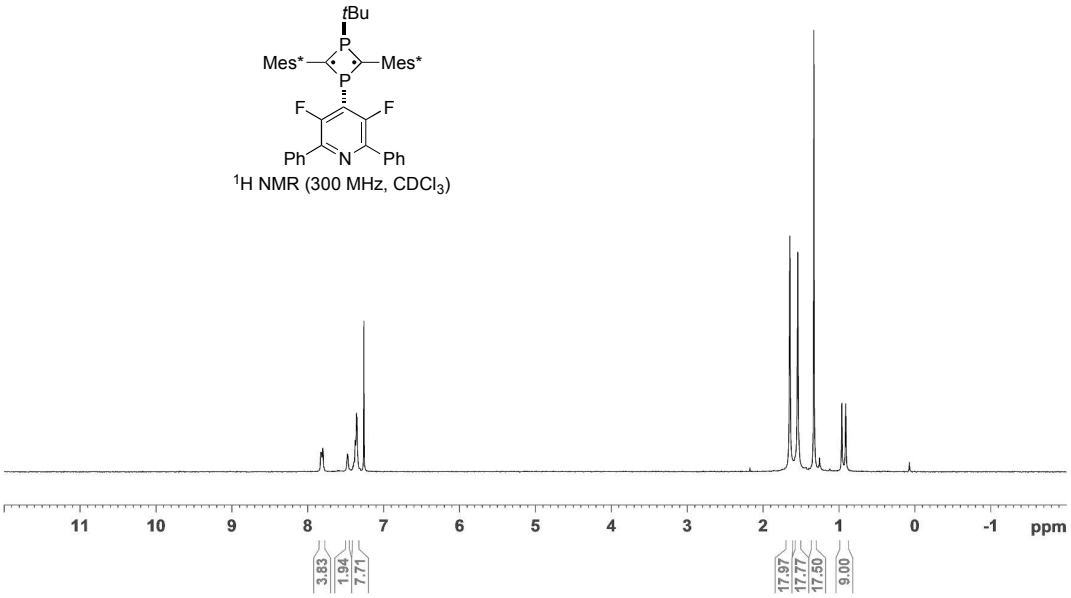


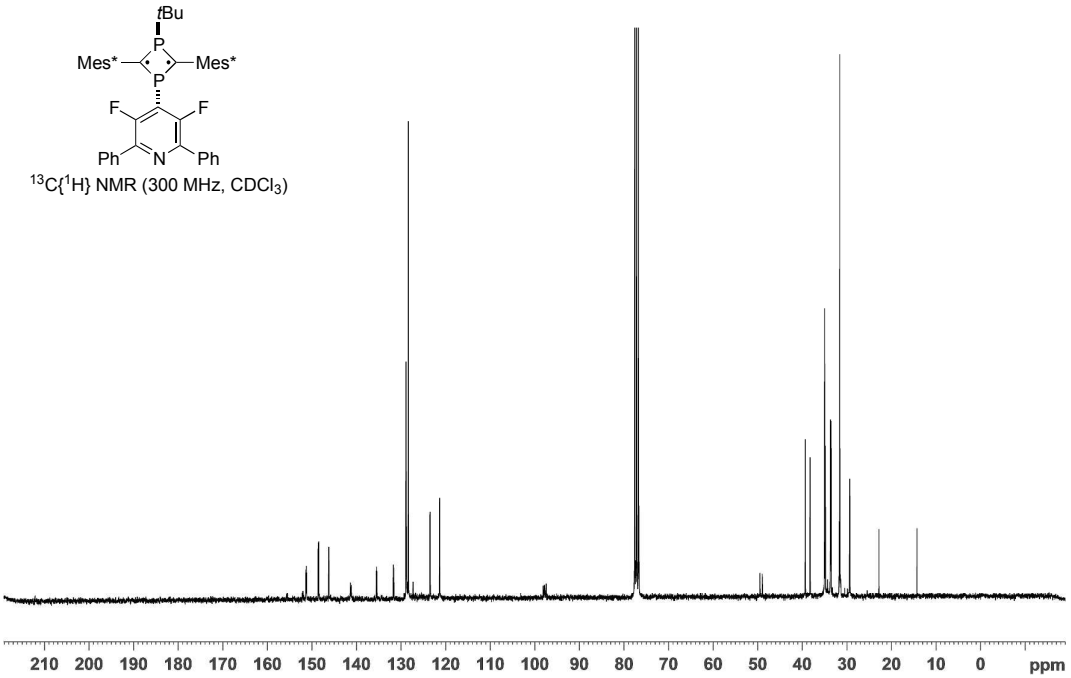
^{19}F NMR (282 MHz, $CDCl_3$)

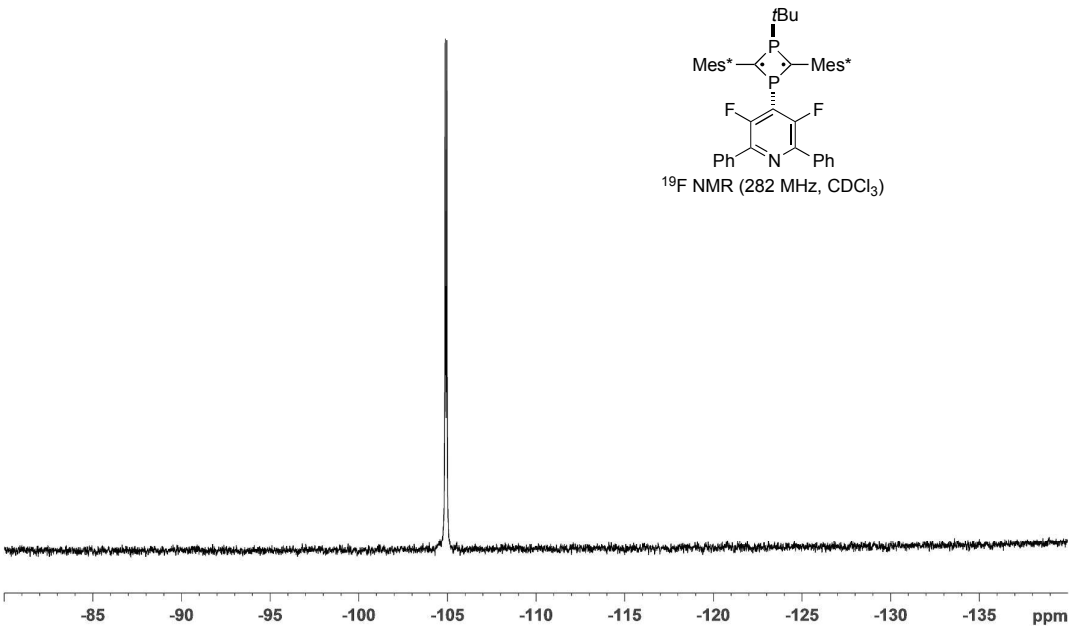


$^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$)

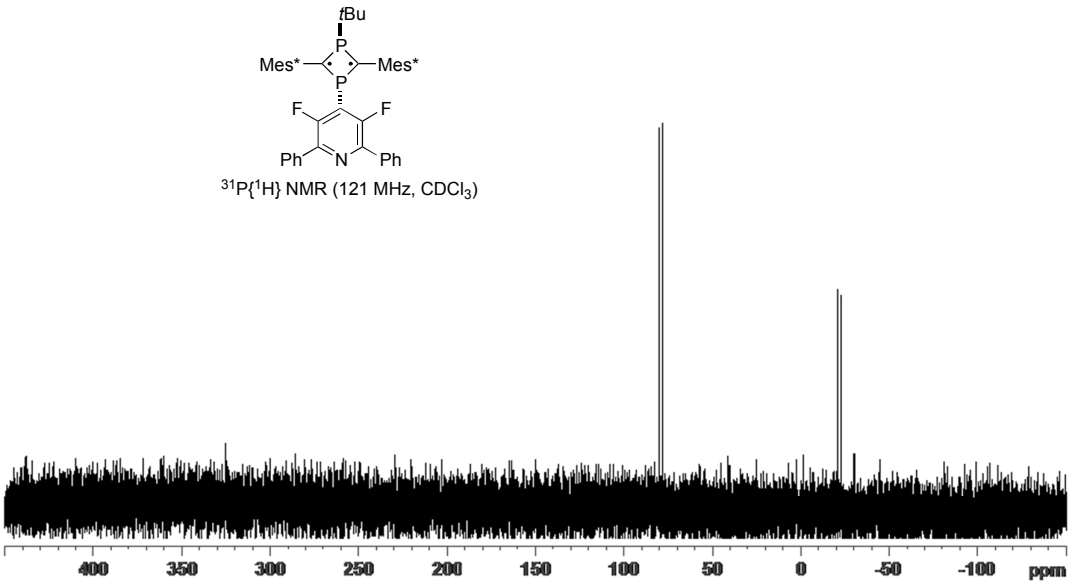
4


tBu
P
Mes*
Mes*
P
F
F
Ph
N
Ph
1H NMR (300 MHz, CDCl3)
11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
3.83
1.94
7.71
17.97
17.77
17.50
9.00


tBu
P
Mes*
Mes*
P
F
F
Ph
N
Ph
13C{1H} NMR (300 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

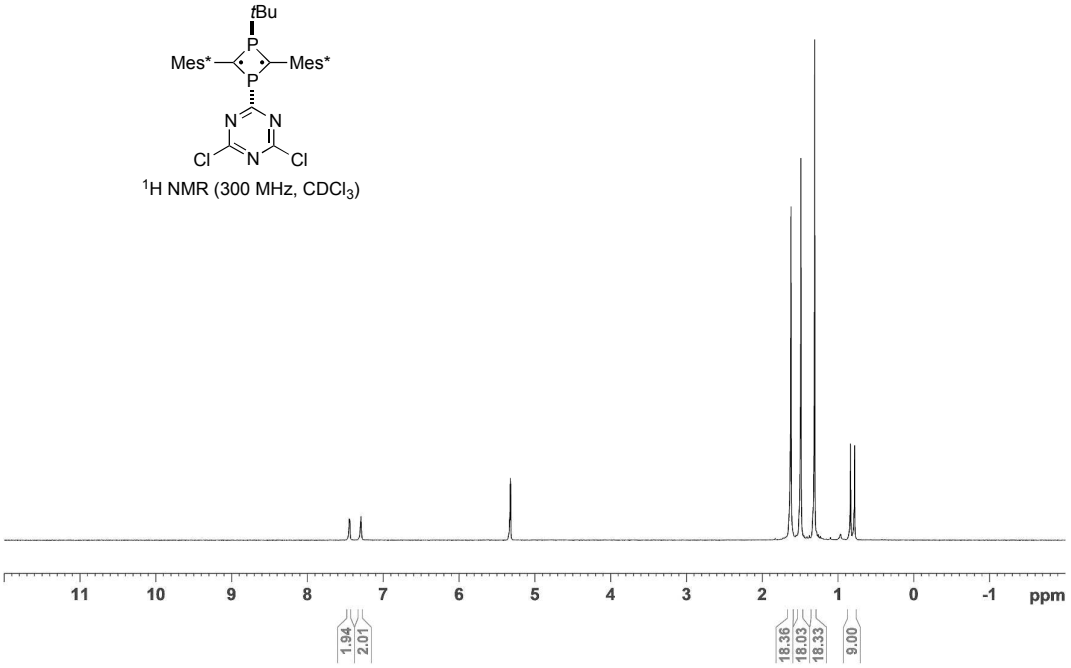


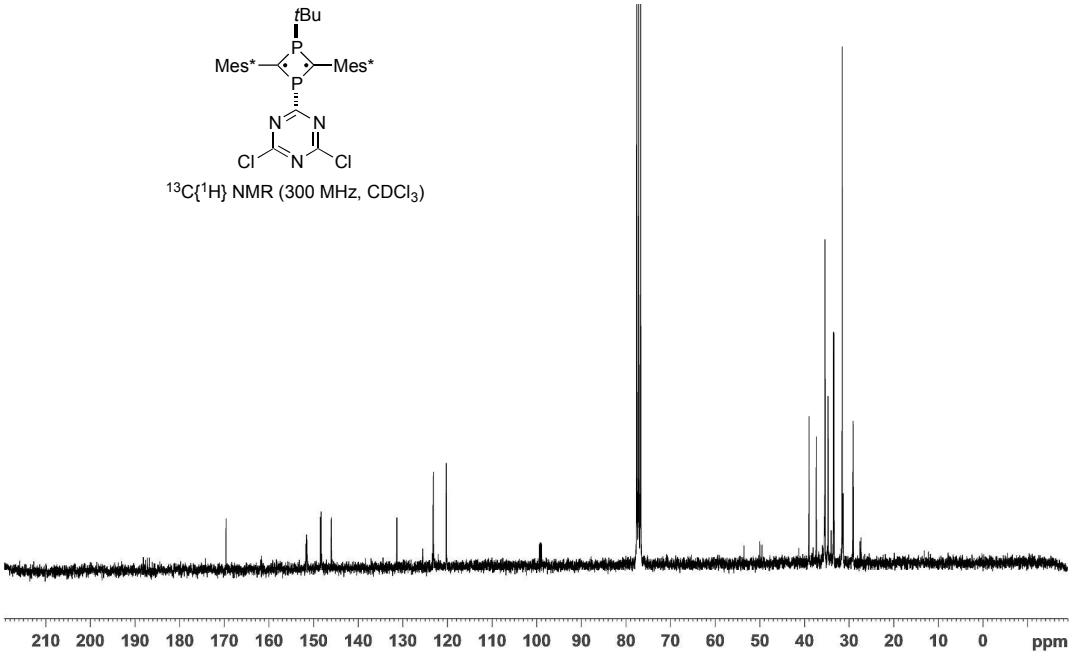
^{19}F NMR (282 MHz, $CDCl_3$)

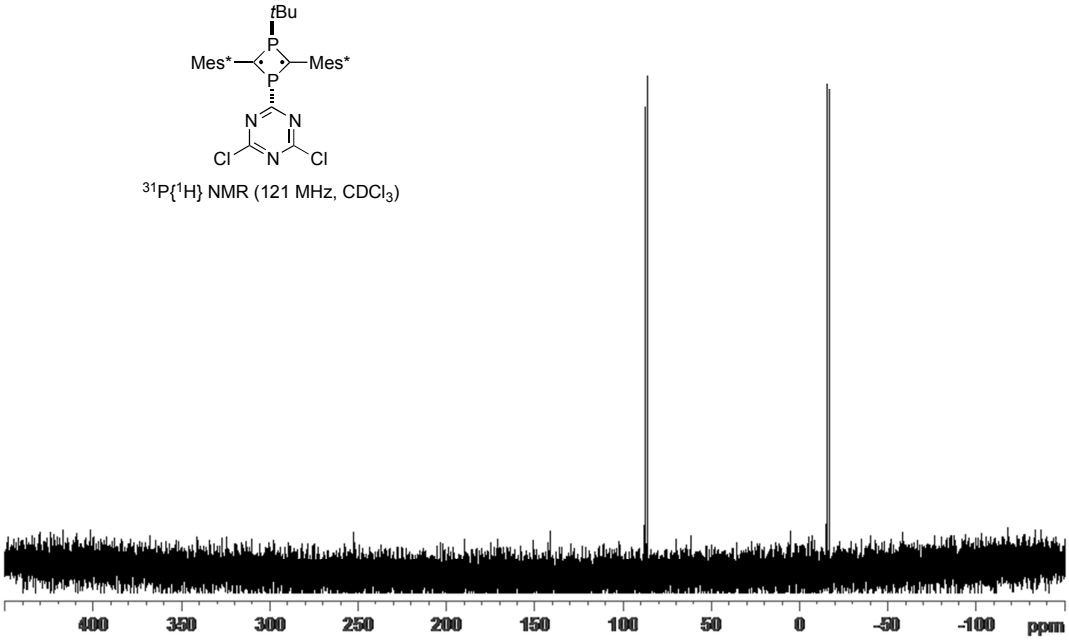


$^{31}P\{^1H\}$ NMR (121 MHz, $CDCl_3$)

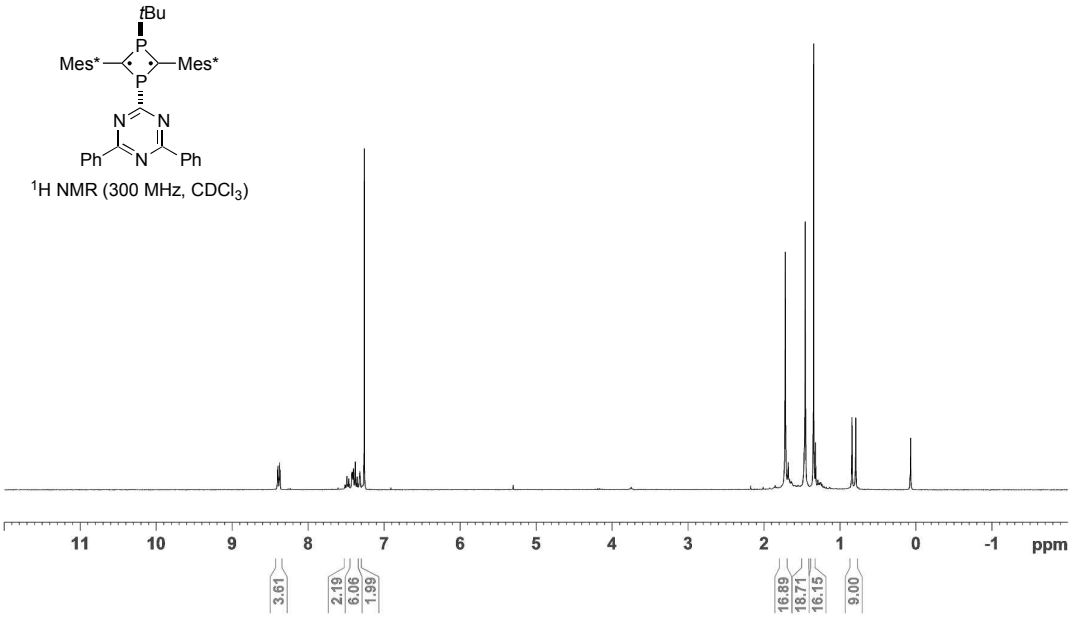
5a

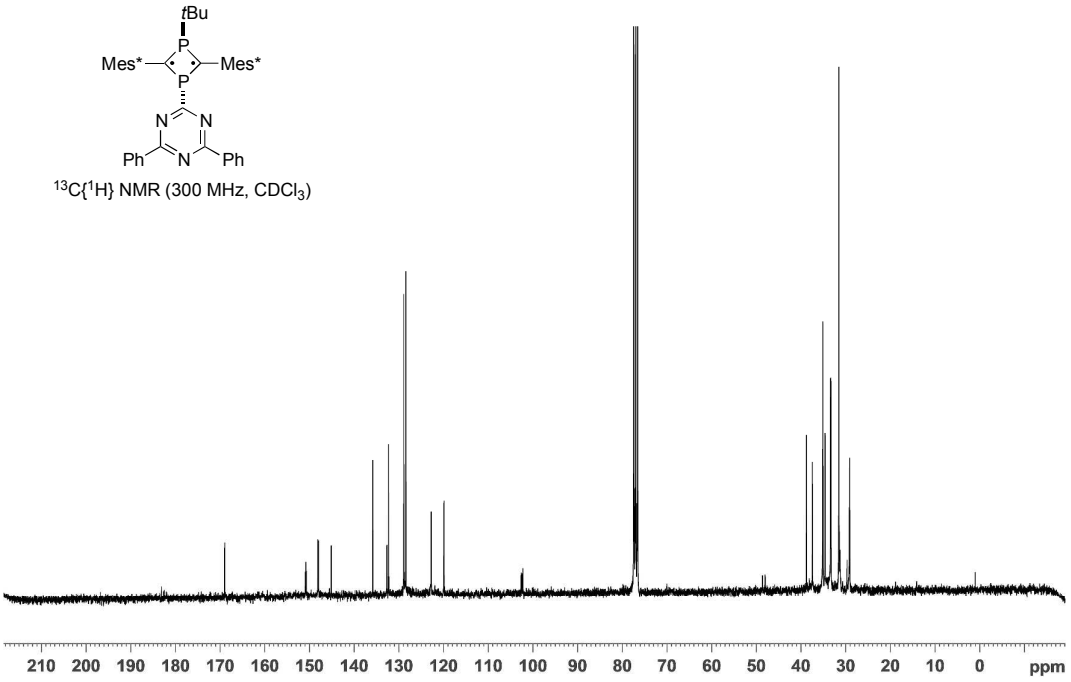

tBu
Mes*
Mes*
Cl
Cl
1H NMR (300 MHz, CDCl3)
11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.94
2.01
18.36
18.03
18.33
9.00


tBu
Mes*
Mes*
Cl
Cl
13C{1H} NMR (300 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

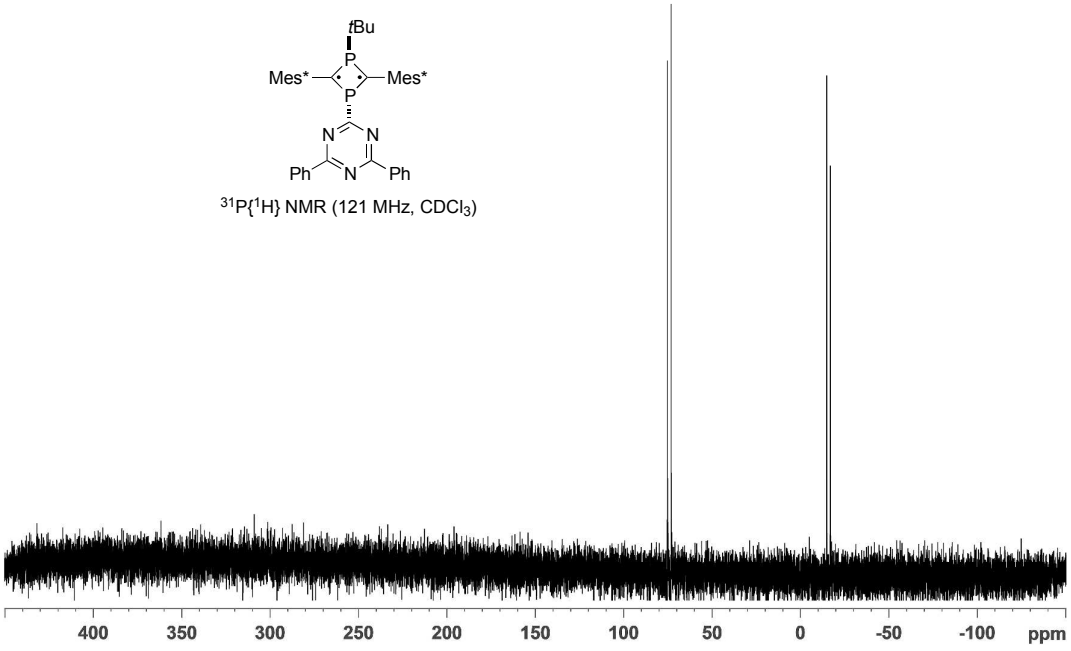

tBu
P
Mes*
Mes*
P
N
N
Cl
N
Cl
31P{1H} NMR (121 MHz, CDCl3)
400
350
300
250
200
150
100
50
0
-50
-100
ppm

5b


tBu
P
Mes*
Mes*
P
N
N
Ph
N
Ph
1H NMR (300 MHz, CDCl3)
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
3.61
2.19
6.06
1.99
16.89
18.71
16.15
9.00

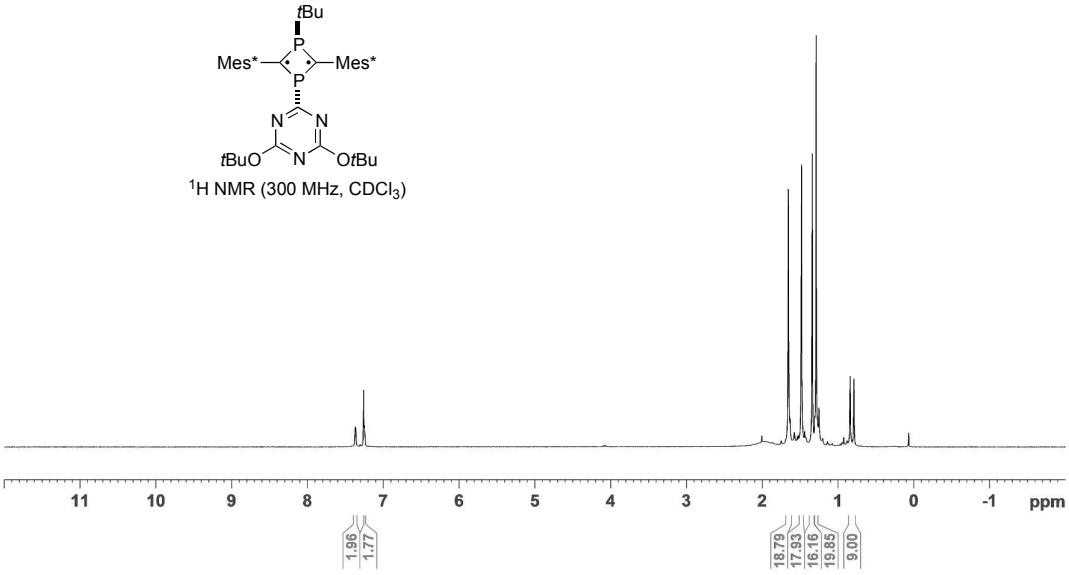


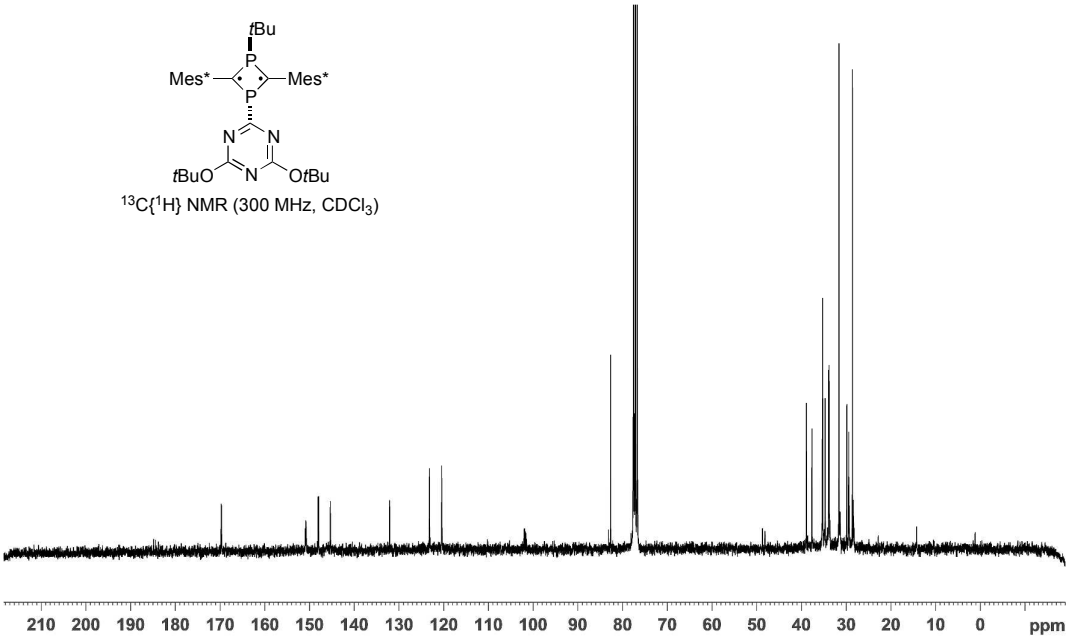
$^{13}C\{^{1}H\}$ NMR (300 MHz, $CDCl_3$)

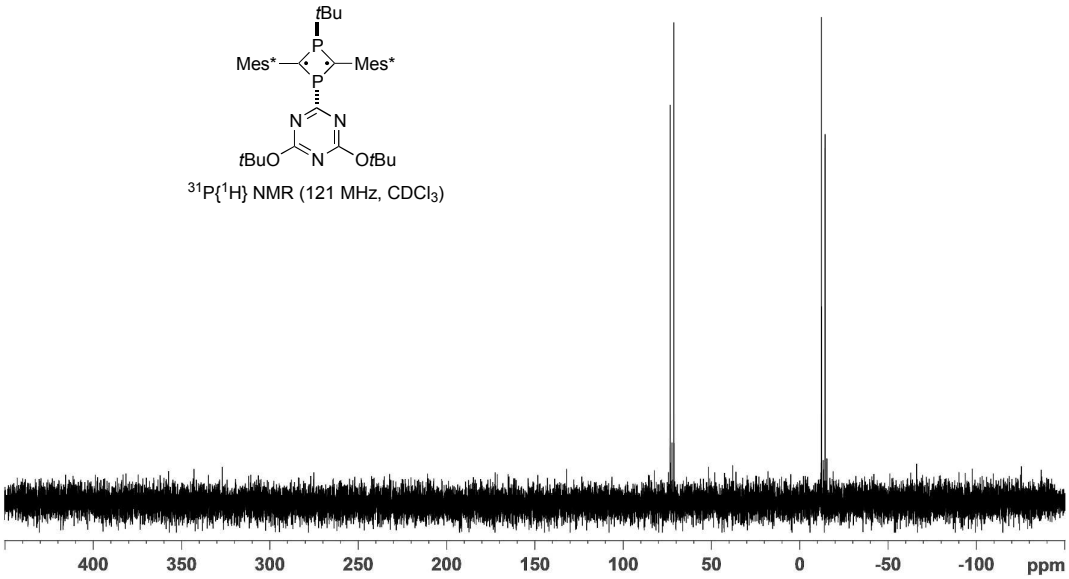


$^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$)

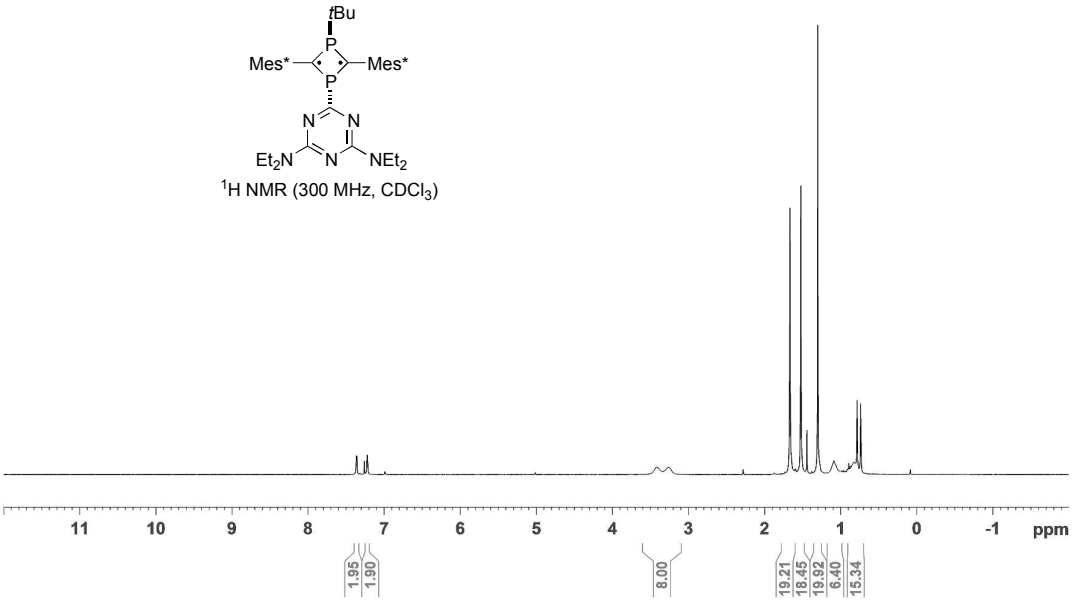
5c

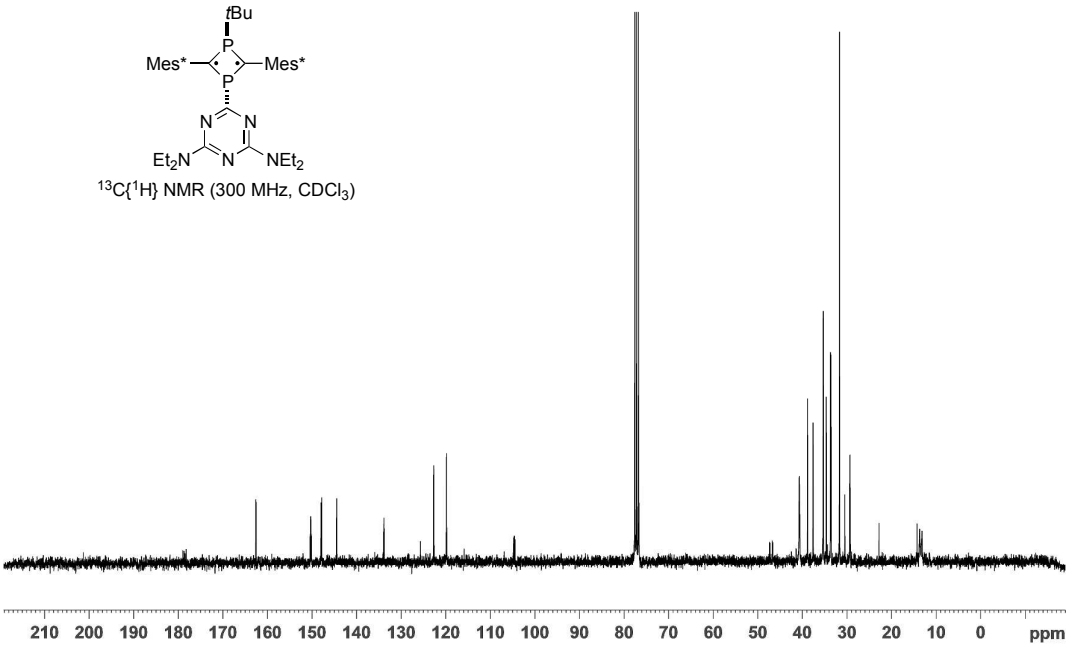

tBu
Mes*
Mes*
tBuO
OtBu
1H NMR (300 MHz, CDCl3)
11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.96
1.77
18.79
17.93
16.16
19.85
9.00


tBu
Mes*
Mes*
tBuO
OtBu
13C{1H} NMR (300 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

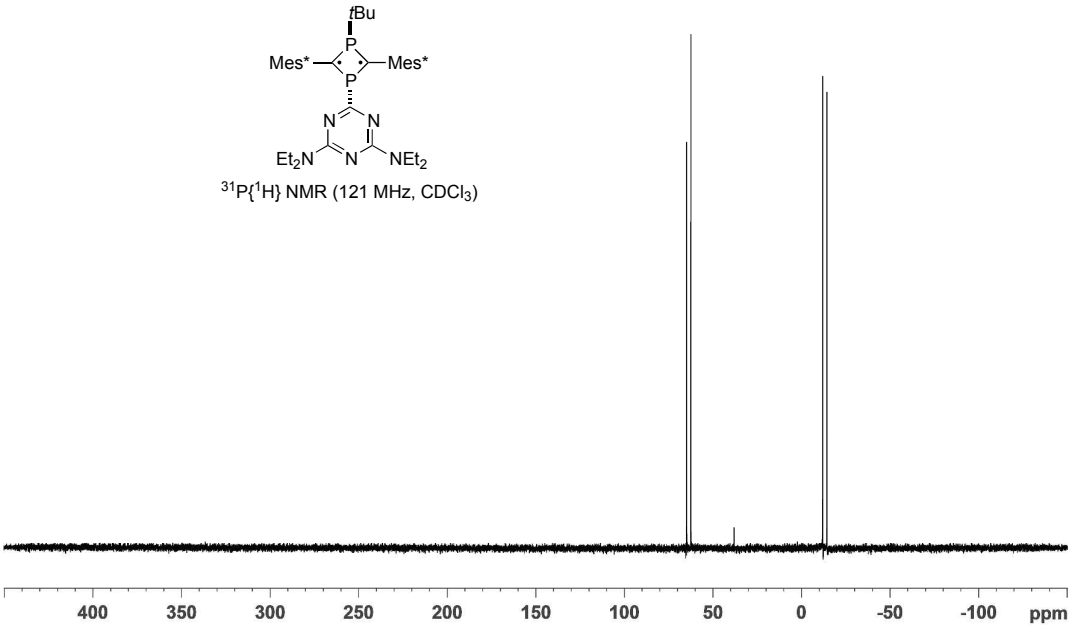

tBu
P
Mes*
Mes*
P
N
N
tBuO
N
OtBu
31P{1H} NMR (121 MHz, CDCl3)
400
350
300
250
200
150
100
50
0
-50
-100
ppm

5d


tBu
P
Mes*
Mes*
P
N
N
Et2N
N
NEt2
1H NMR (300 MHz, CDCl3)
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.95
1.90
8.00
19.21
18.45
19.92
6.40
15.34

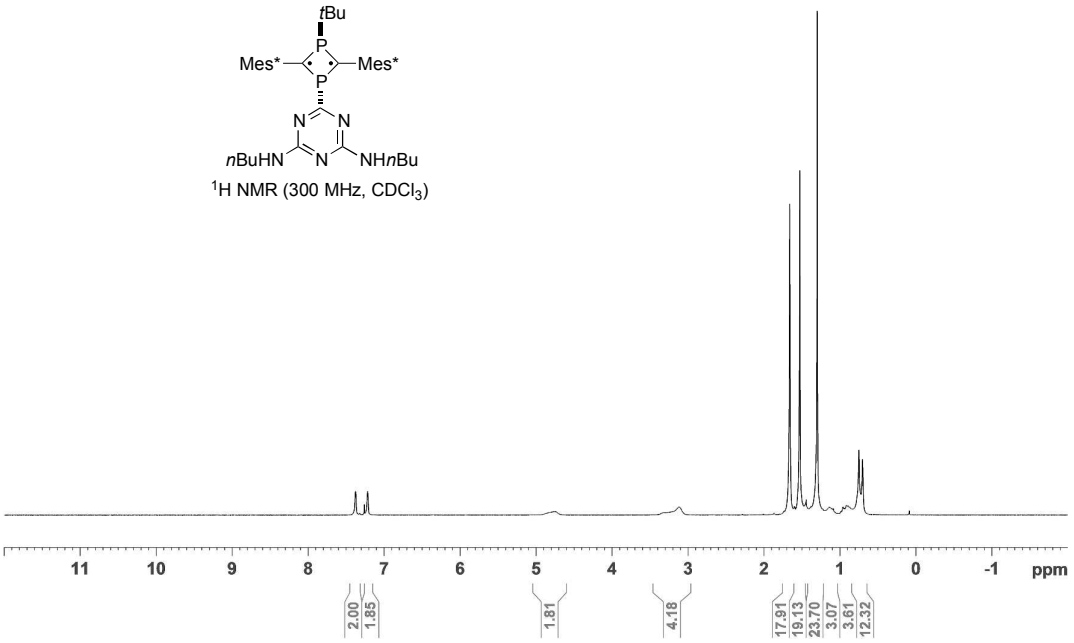


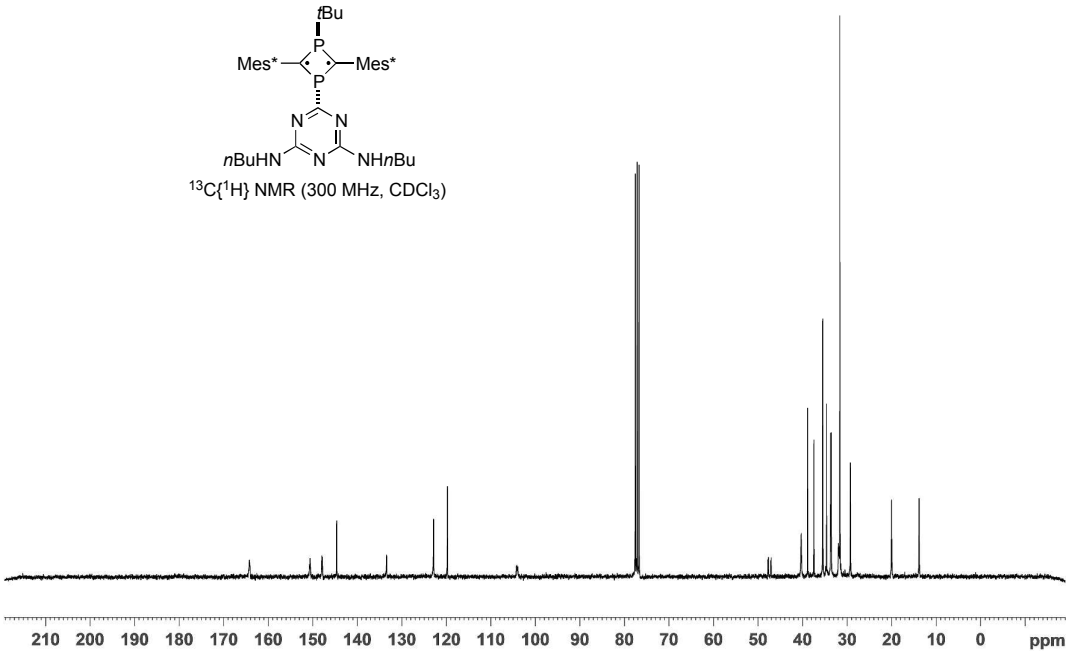
$^{13}C\{^{1}H\}$ NMR (300 MHz, $CDCl_3$)

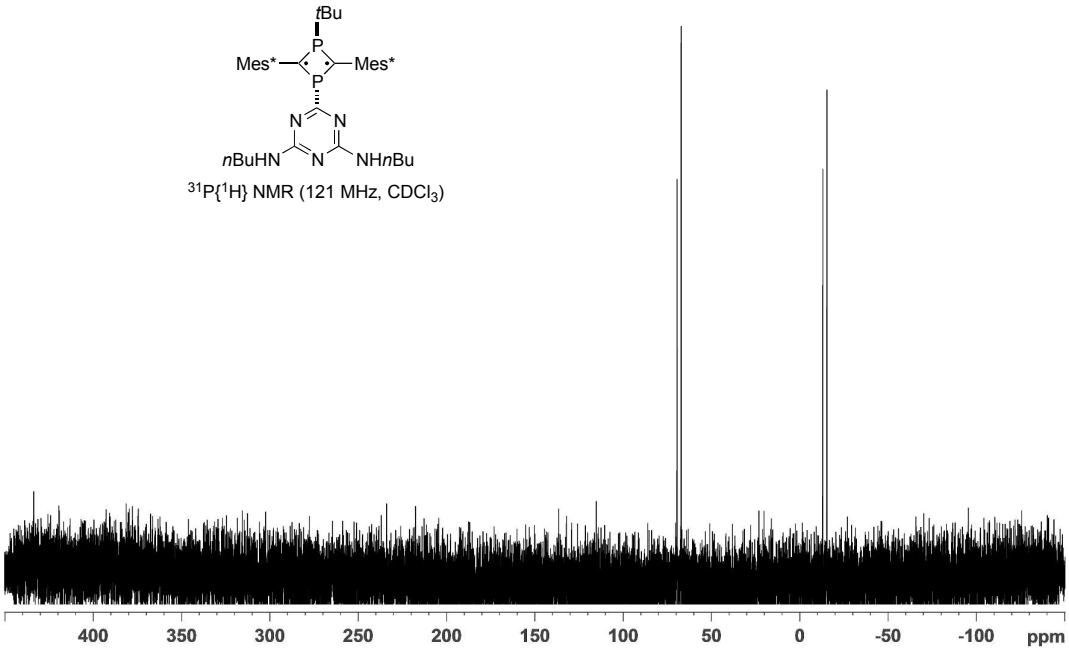


$^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$)

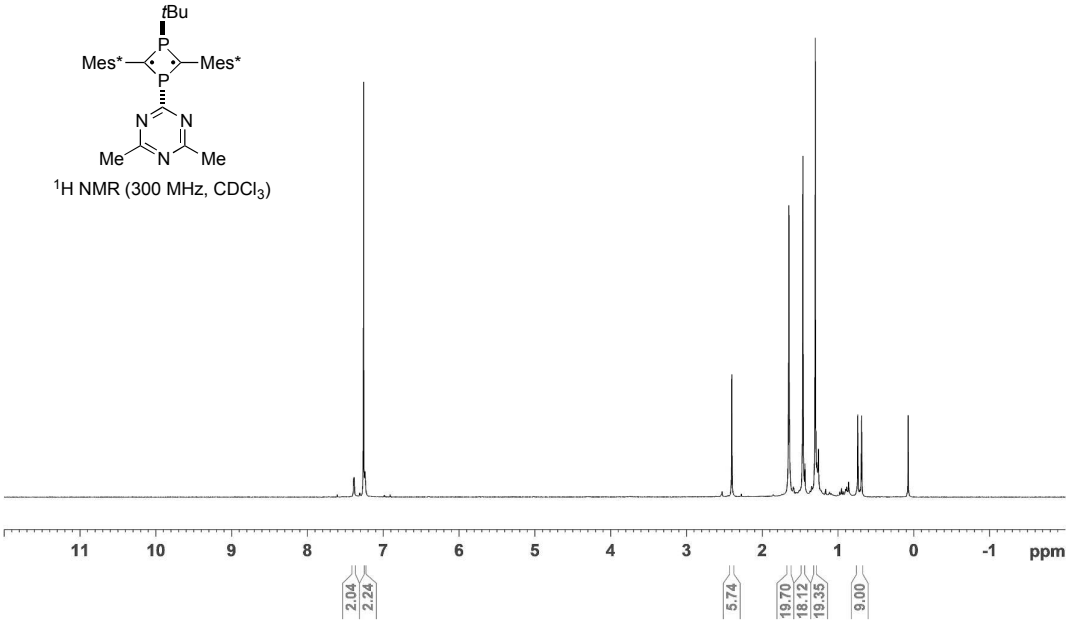
5e

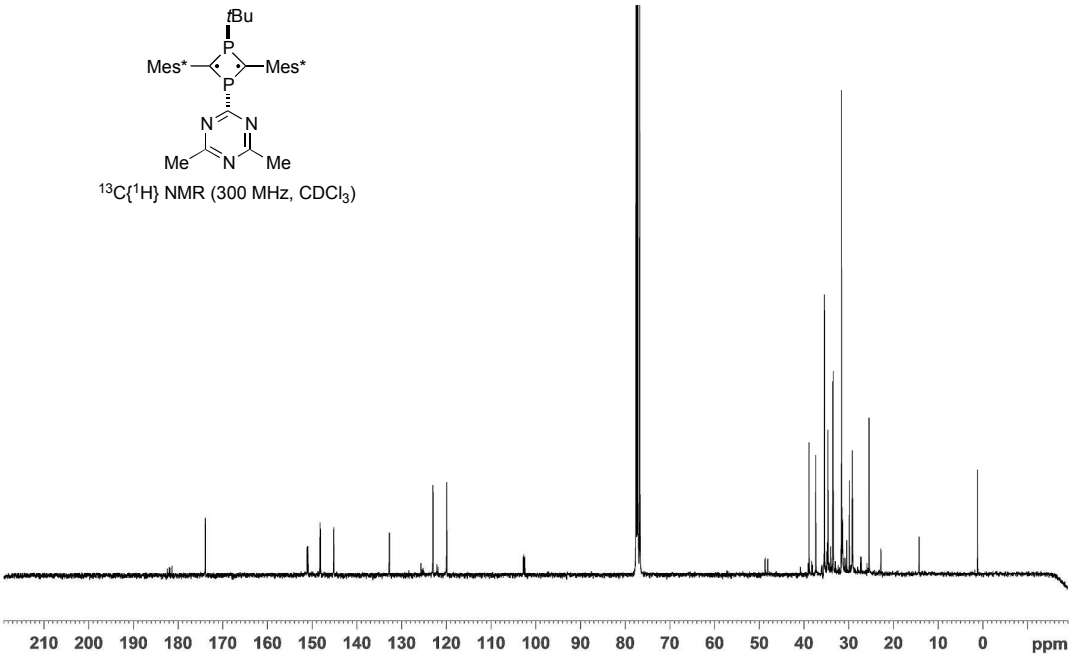

tBu
Mes*
Mes*
nBuHN
NHnBu
1H NMR (300 MHz, CDCl3)
11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
2.00
1.85
1.81
4.18
17.91
19.13
23.70
3.07
3.61
12.32


tBu
Mes*
Mes*
nBuHN
NHnBu
13C{1H} NMR (300 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

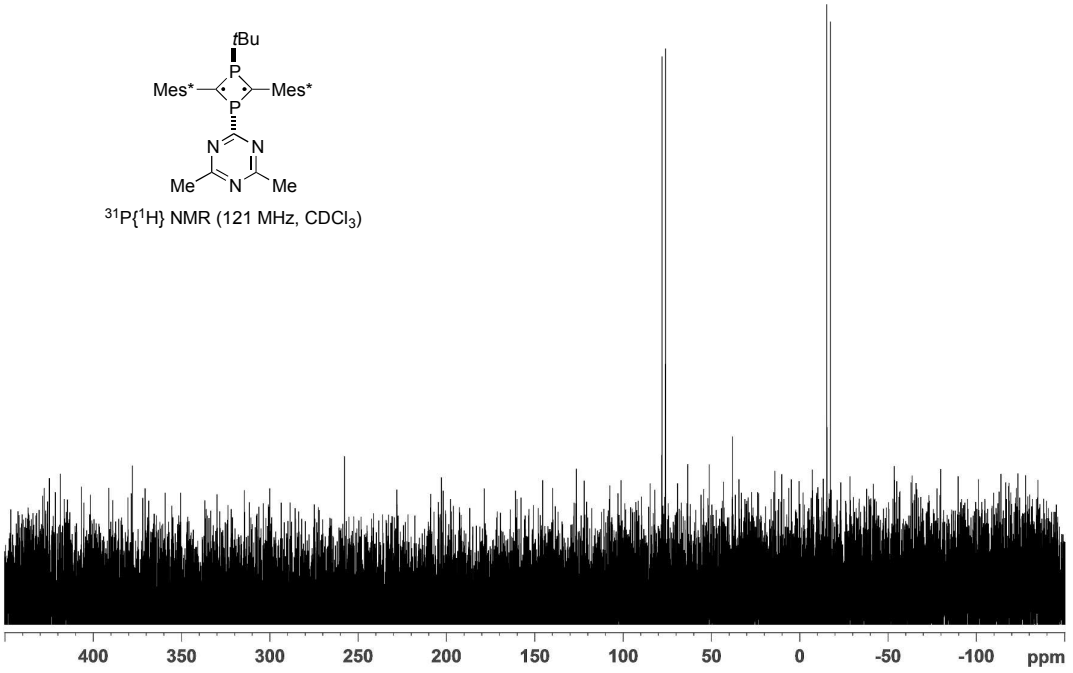

tBu
Mes*
Mes*
nBuHN
NHnBu
31P{1H} NMR (121 MHz, CDCl3)
400
350
300
250
200
150
100
50
0
-50
-100
ppm

5f


tBu
Mes*
Mes*
Me
Me
1H NMR (300 MHz, CDCl3)
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.04
2.24
5.74
19.70
18.12
19.35
9.00

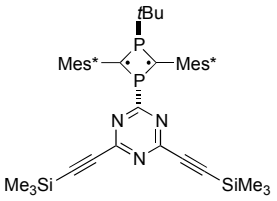


$^{13}C\{^{1}H\}$ NMR (300 MHz, $CDCl_3$)

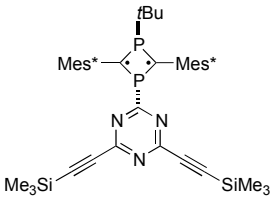


$^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$)

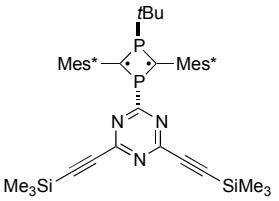
5g



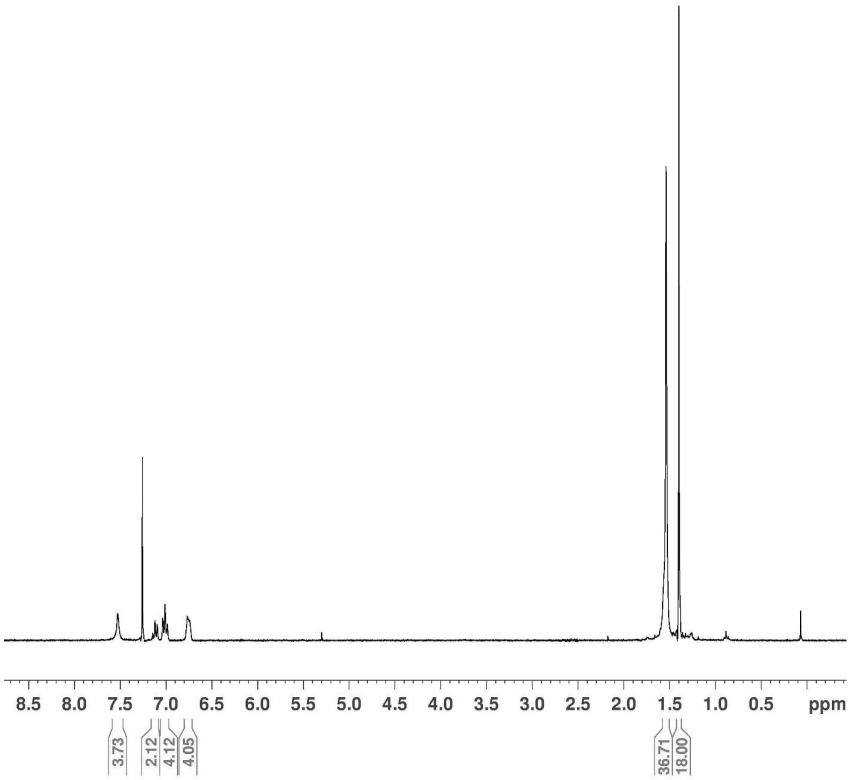
^{1}H NMR (300 MHz, $CDCl_3$)



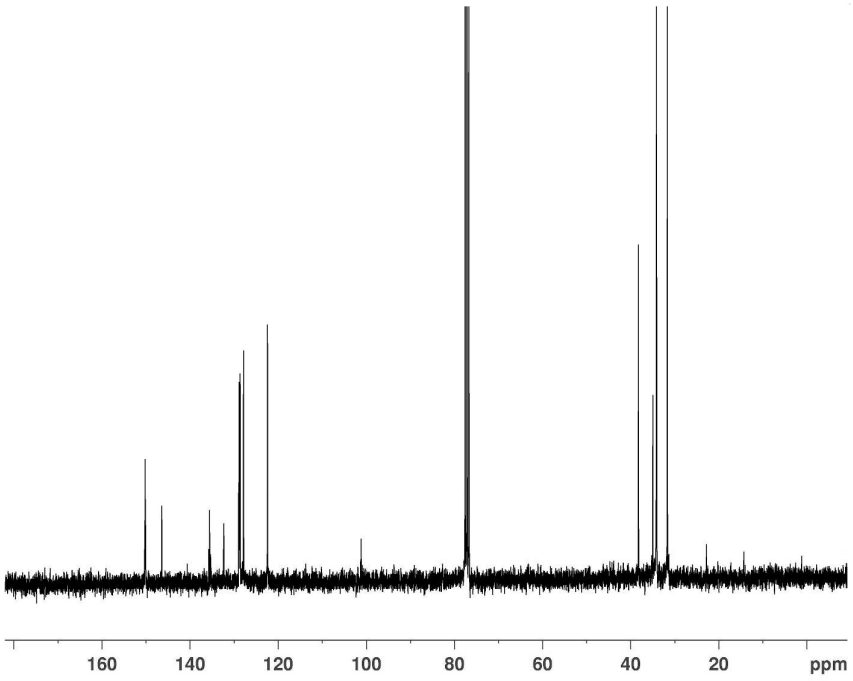
^{13}C{^{1}H} NMR (300 MHz, $CDCl_3$)



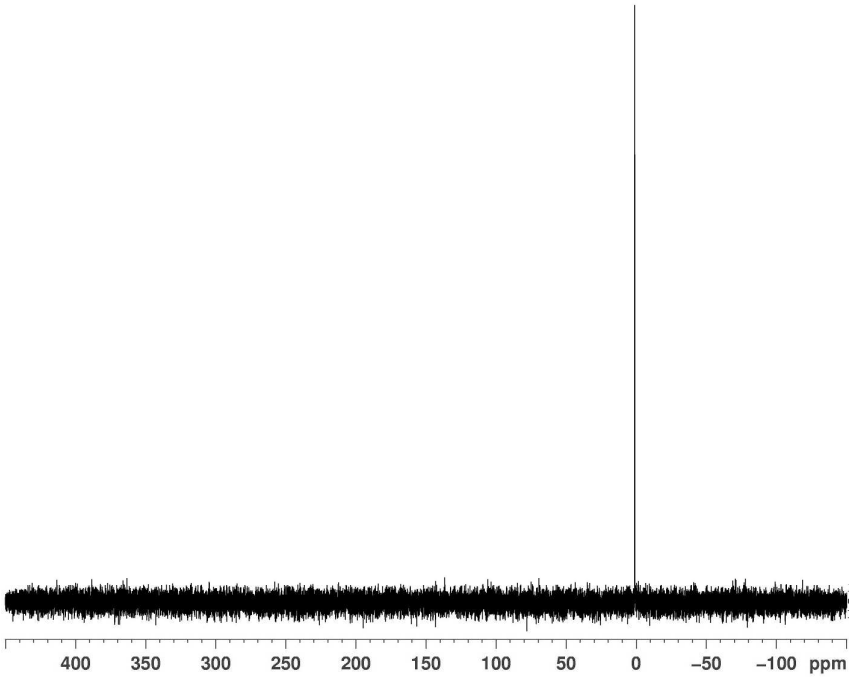
$^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$)



^{1}H NMR (300 MHz, $CDCl_3$) of **7**



$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) of **7**



$^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$) of **7**

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