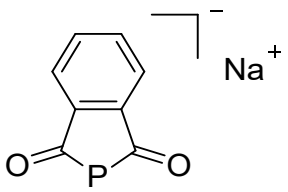
# Supporting Information



## S1: Synthetic Details

**General:** All manipulations were performed under an inert atmosphere of dry nitrogen, using standard Schlenk techniques. Dry, oxygen-free solvents were employed unless otherwise mentioned. The compound **2** were prepared following literature procedures,[1] while all other starting materials were purchased from commercial sources except otherwise mentioned. NMR spectra were recorded on Bruker Avance 400 or 300 MHz spectrometers. All spectra were obtained in the solvent indicated at 25 °C. $^{1}H$ and $^{13}C$ NMR spectra in $CDCl_3$ were referenced internally to $SiMe_4$ and in other deuterated solvents were referenced to the internal residual solvent chemical shifts. $^{31}P$ NMR spectra were referenced externally to 85% $H_3PO_4$. Coupling constants *J* are reported in Hertz [Hz] as absolute values. The elemental analyses were acquired on Vario EL cube elemental analyzer. IR spectra were obtained on a Perkin-Elmer-Spectrum ATR 2000 FT-IR-Raman spectrometer with KBr beam splitter (range 500 – 4000 $cm^{-1}$ ).




**1[Na]**

**Preparation of Sodium Isophosphindolin-1,3-dionide (Sodium Phosphaphthalimid)** (**1[Na]**): A literature method was modified.[2] A 1 L round-bottom Schlenk flask was flushed with dinitrogen and charged with red phosphorus (6.2 g, 0.2 mol, 1 eq.) and naphthalene (2.56 g, 0.1 eq.). Tetrahydrofuran (THF) (600 ml) was added to the flask. Subsequently, sodium (13.8 g, 0.6 mol, 3 eq.) was added to the suspension as 1 cm nuggets. The formation of black sodium phosphide particles ($Na_3P$) is immediately apparent. After stirring the mixture for 12 hours at 55 °C, it was cooled to 10 °C in a water bath. Degassed tert-butanol (14.82 g, 19.13 ml, 1eq.) solution in THF (20 ml) was added drop-wise to the black suspension of $Na_3P$ over a period of 30 min. After stirring the reaction mixture for one hour, it was cooled down to 0 °C using an ice-water bath. Degassed diethyl phthalate (48.89 g, 43.73 ml, 0.22 mol, 1.1 eq.) solution in THF (40 ml) was added drop-wise over a period of 1 hour at 0 °C. The color of the reaction mixture turned immediately to a deep burgundy red. Subsequently, the reaction was warmed to ambient temperature and stirred for 1 hour at room temperature. After stirring at 55 °C for another 12 hours, the reaction mixture was filtered. Then the volume of the reaction mixture was reduced to about 200 ml at 55 °C. Then, let it cool to RT slowly without stirring, lots of crystals precipitate within 2 hours, and afterwards stored it at –20 °C for another 12 hours. The deep burgundy red crystals were collected by filtration, washed with *n*-hexane (20 ml), and dried under vacuum (41.2 g, yield 78.3 %). According to NMR spectrum, this solid has the composition [**1**·$(THF)_{1.1}$]. Deep burgundy red single crystals of [**1**·$(THF)_3$] were obtained after slow evaporation of **1** in saturated THF solution. M.P. = 212 °C (Decomposition). $^1$H NMR (400 MHz, $CD_3CN$): δ = 7.91 (m, 4H, $C_{ar}H^3$), 3.65 (m, 4H, $OCH_2$, thf), 1.81 (m, 4H, $OCH_2CH_2$, thf). $^{13}$C{H} NMR (100.5 MHz, $CD_3CN$): δ = 206.1 (d, $J_{CP}$ = 70.4 Hz, *C*OP*C*O), 136.4 (s, $C_{ar}$), 134.6 (d, $J_{CP}$ = 50.3 Hz, $C_{ar}$), 123.5 (s, $C_{ar}$), 67.3 (s, $OCH_2$, thf), 25.2 (s, $OCH_2CH_2$, thf). $^{31}$P{H} NMR (161.9 MHz, $CD_3CN$): δ = 22.0 (s). Elemental analysis (%): calcd for $C_{12}H_{12}O_3P$; C 55.82, H 4.68; found: C 55.13, H 4.96. **IR** (ATR, [$cm^{-1}$]): 1474.2 (C=O).

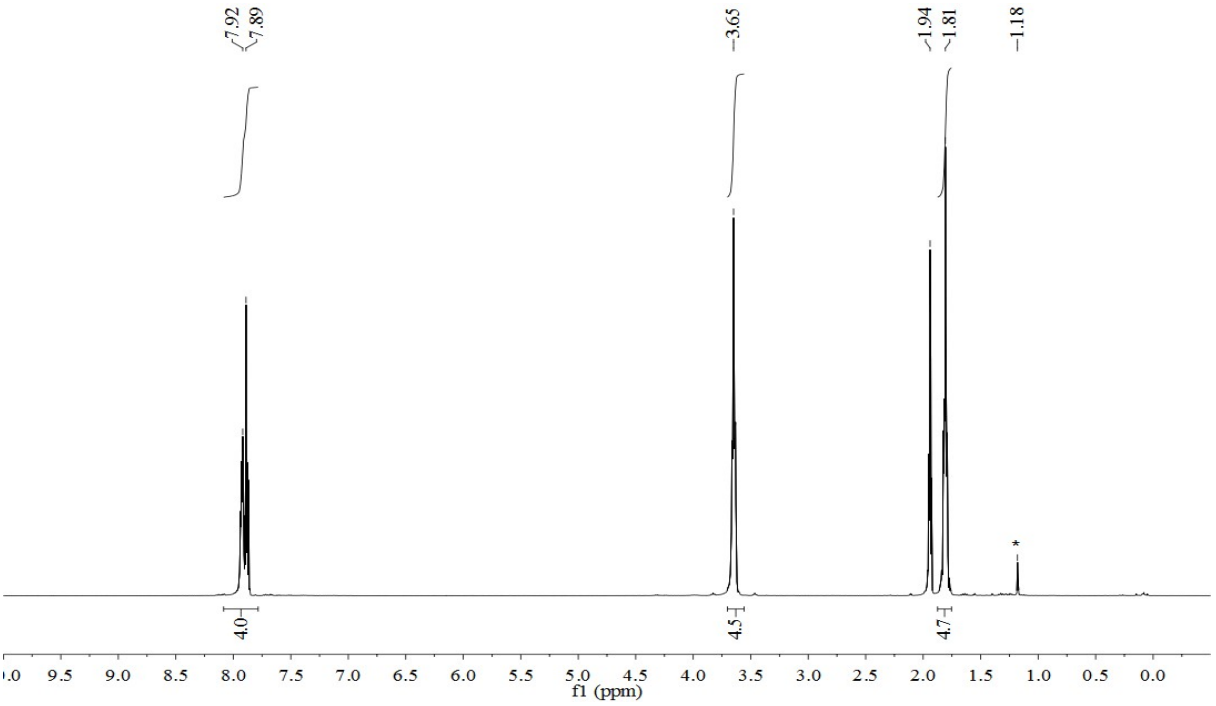



***Figure S1.*** $^{1}H$ NMR spectrum of **1** in $CD_3CN$. *Tert-butoxide.

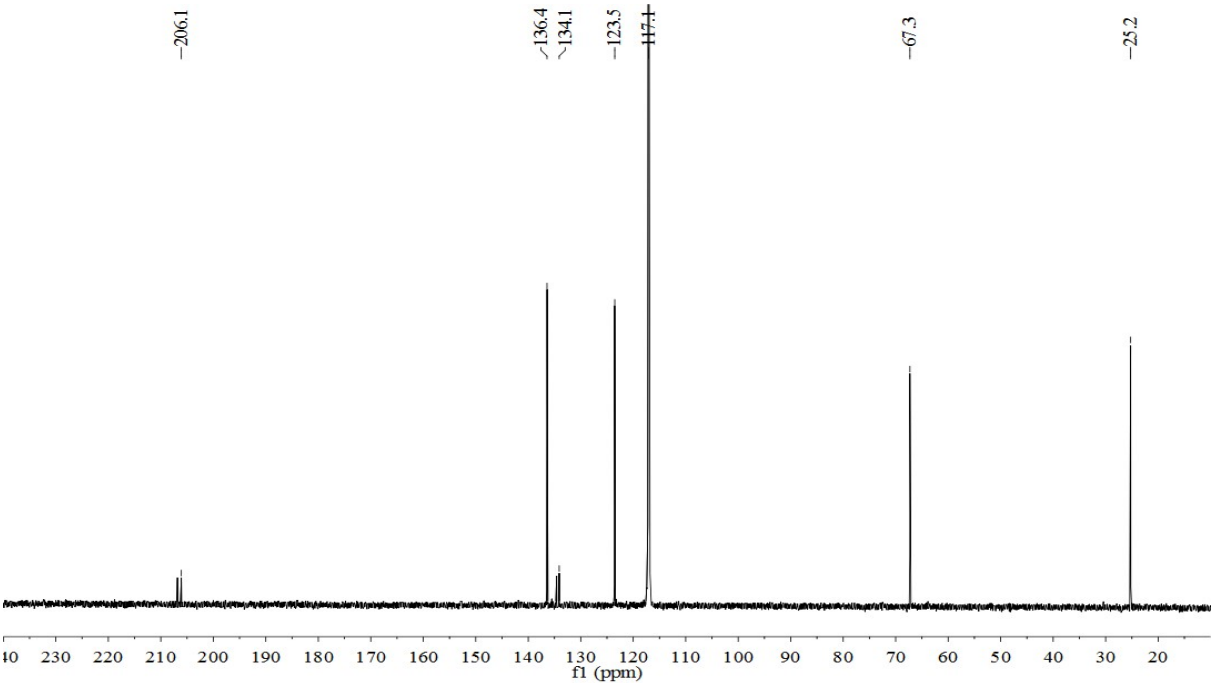



***Figure S2.*** $^{13}C\{^{1}H\}$ NMR spectrum of **1** in $CD_3CN$.

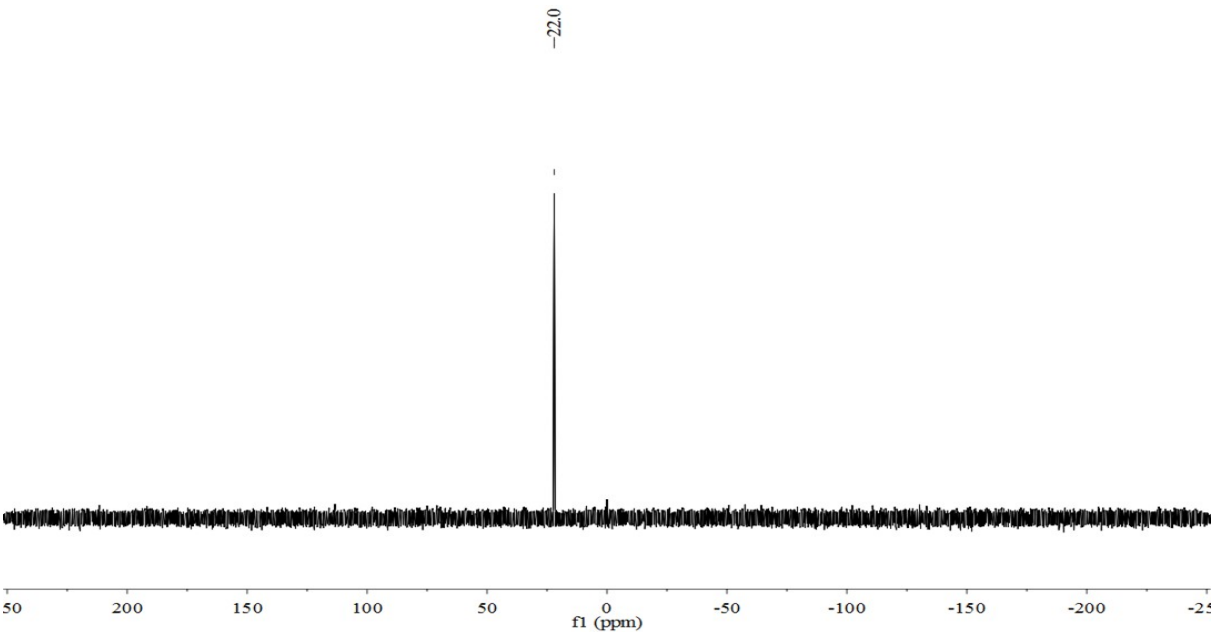



***Figure S3.*** $^{31}P\{^{1}H\}$ NMR spectrum of **1** in $CD_3CN$.

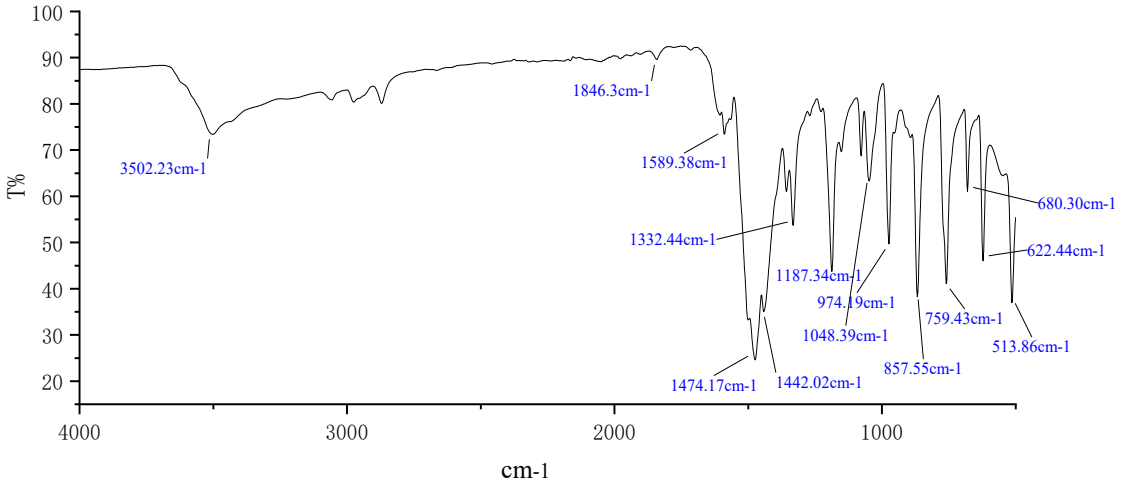
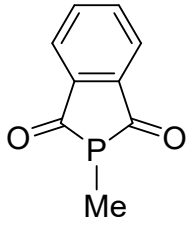



***Figure S4.*** IR spectrum of **1**




**1**-Me

**Preparation of 2-methyl-isophosphindoline-1,3-dione** (**1**-Me): Iodomethane (71.0 mg, 0.5 mmol) in THF (2 mL) was added dropwise to a stirred solution of **1** (1.2 equivalent) in THF (4 mL). After stirring for 2 hours, the solvent was removed under reduced pressure. The remaining residue was extracted with dichloromethane, then the solvent was removed under reduced pressure. The remaining solid was dried *in vacuo* affording a yellow powder **6** (81.3 mg, 0.46 mmol, 91.3 % yield). M. P. = 68 °C. $^{1}$H NMR (400 MHz, $CDCl_3$): δ = 7.82 (m, 2H, $C_{ar}H$), 7.74 (m, 2H, $C_{ar}H$), 1.51 (s, 3H, $CH_3$). $^{13}$C{H} NMR (100.5 MHz, $CDCl_3$): δ = 215.1 (d, $J_{CP}$ = 35.7 Hz, *C*O), 114.9 (d, $J_{CP}$ = 27.3 Hz, $C_{ar}$), 134.4 (s, $C_{ar}$), 121.2 (s, $C_{ar}$), 4.2 (d, $J_{CP}$ = 27.0 Hz, $CH_3$). $^{31}$P{H} NMR (161.9 MHz, $CDCl_3$): δ = –34.9 (s). Elemental analysis (%): calcd for $C_9H_7O_2P$; C 60.67, H 3.96; found: C 60.11, H 4.18. **IR** (ATR, [$cm^{-1}$]): 1649.2 (C=O).

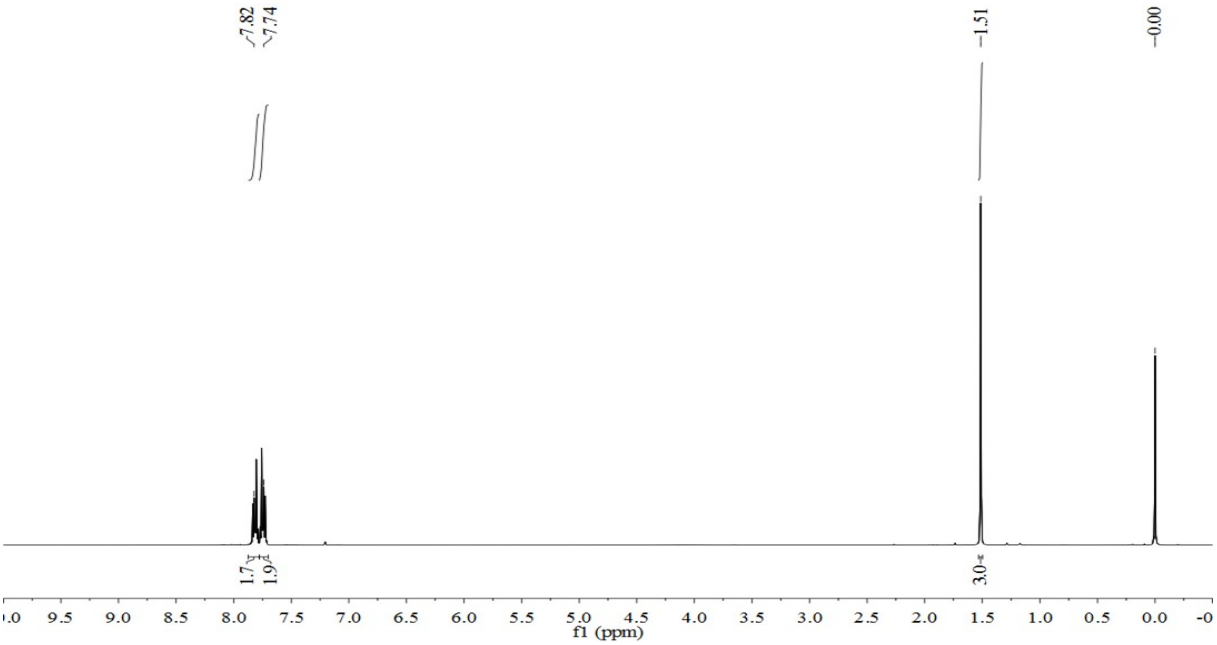



***Figure S5.*** $^{1}$H NMR spectrum of **1-Me** in $CDCl_3$.

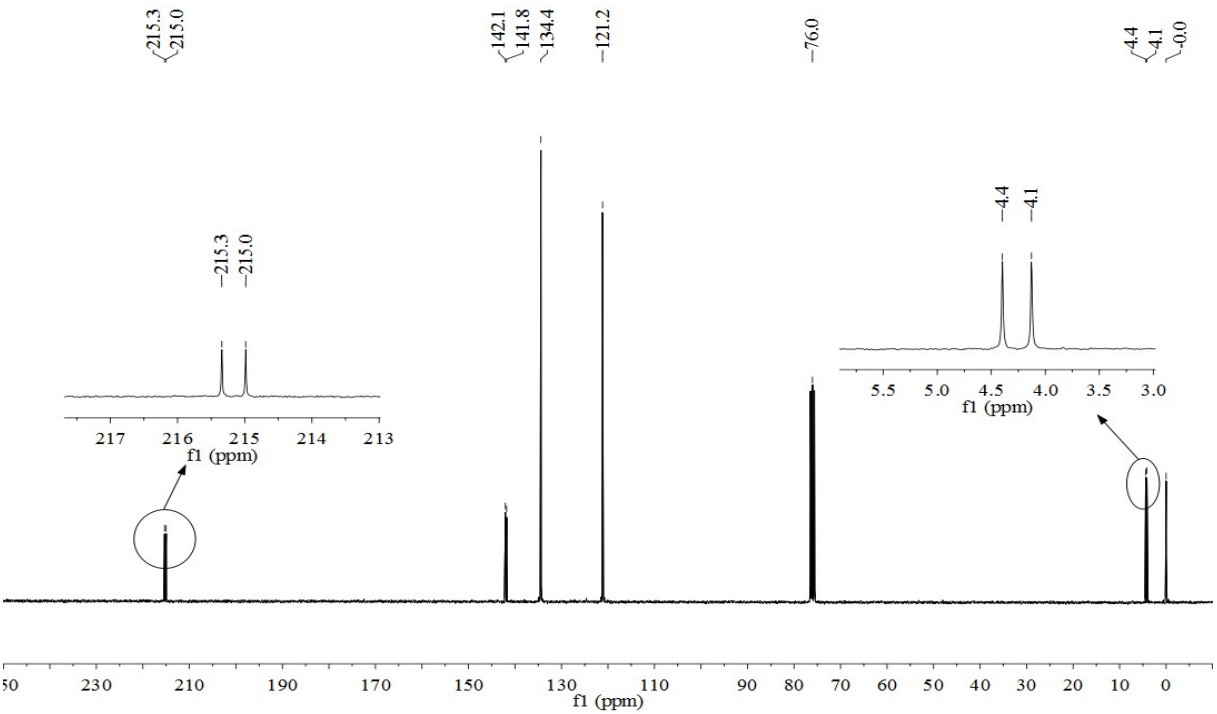



***Figure S6.*** $^{13}C\{^{1}H\}$ NMR spectrum of **1-Me** in $CDCl_3$.

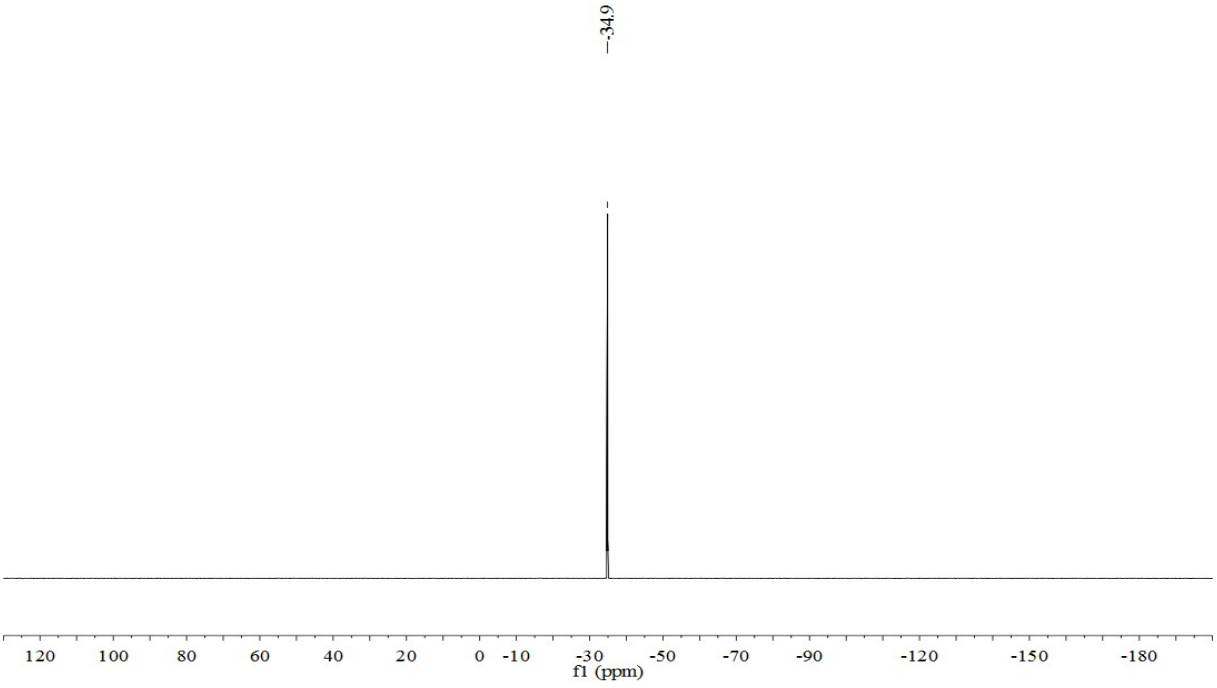



***Figure S7.*** $^{31}P\{^{1}H\}$ NMR spectrum of **1-Me** in $CDCl_3$.

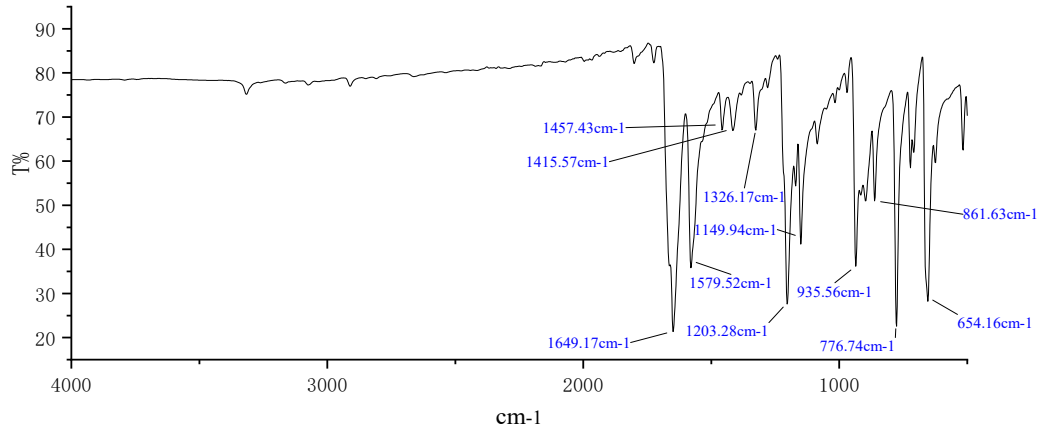
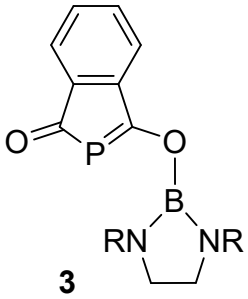



***Figure S8.*** IR spectrum of **1**-Me




**3**

**Preparation of 3:** 1,3-bis(2,6-diisopropylphenyl)-2-bromo-1,3,2-diazaborolidine (**2**) (235.0 mg, 0.5 mmol) in THF (4 mL) was added dropwise to a stirred solution of **1** (1.2 equivalent) in THF (4 mL). After stirring for 1 hour, the solvent was removed under reduced pressure. The remaining residue was extracted with dichloromethane, then the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* affording a red powder **3** (221.6 mg, 0.40 mmol, 80.2 % yield). Red crystals of **3** were obtained from a saturated solution of hexane and THF via slow evoporation. M. P. = 194 °C. $^{1}$H NMR (400 MHz, $C_6D_6$): δ = 7.07 (m, 7H, $C_{ar}H$), 6.88 (d, 1H, $J$ = 7.2 Hz, $C_{ar}H$), 6.56 (t, 1H, $J$ = 7.6 Hz, $C_{ar}H$), 6.49 (t, 1H, $J$ = 7.2 Hz, $C_{ar}H$), 3.66 (m, 4H, $CH$Me$_2$), 3.53 (m, 4H, $CH_2$), 1.37 (d, 12H, $J$ = 6.8 Hz, $CH_3$), 1.26 (d, 12H, $J$ = 6.8 Hz, $CH_3$). $^{13}$C{H} NMR (100.5 MHz, $C_6D_6$): δ = 220.9 (d, $J_{CP}$ = 52.5 Hz, *C*OPCOB), 216.6 (d, $J_{CP}$ = 52.4 Hz, COP*C*OB), 146.9 (s, $C_{ar}$), 144.4 (d, $J_{CP}$ = 12.9 Hz, $C_{ar}$), 137.3 (s, $C_{ar}$), 136.9 (d, $J_{CP}$ = 7.3 Hz, $C_{ar}$), 132.5 (d, $J_{CP}$ = 3.4 Hz, $C_{ar}$), 129.8 (d, $J_{CP}$ = 6.2 Hz, $C_{ar}$), 124.0 (s, $C_{ar}$), 120.2 (s, $C_{ar}$), 116.8 (d, $J_{CP}$ = 10.2 Hz, $C_{ar}$), 51.5 (s, $CH_2$), 28.5 (s, *C*HMe$_2$), 25.2 (s, $CH_3$), 24.5 (s, $CH_3$). $^{31}$P{H} NMR (161.9 MHz, $C_6D_6$): δ = 79.5 (s). Elemental analysis (%): calcd for $C_{34}H_{42}N_2O_2PB$; C 73.87, H 7.66; found: C 73.54, H 7.94. **IR** (ATR, [cm$^{-1}$]): 1669.8 (C=O).

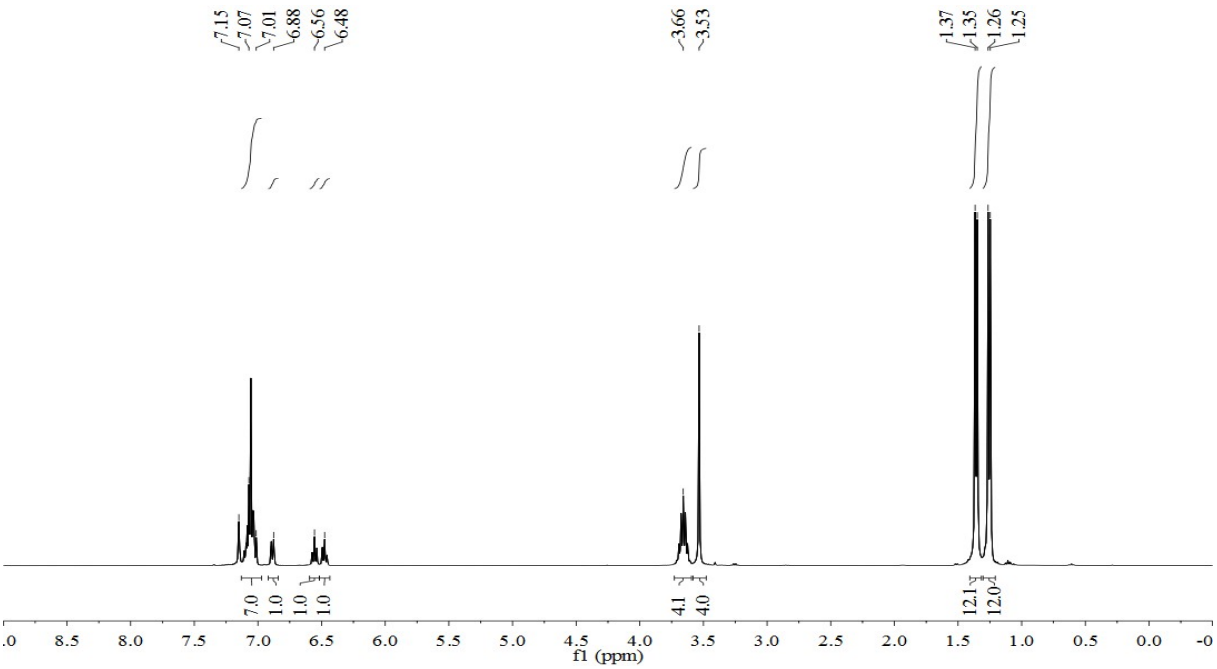



***Figure S9.*** $^{1}$H NMR spectrum of **3** in $C_6D_6$.

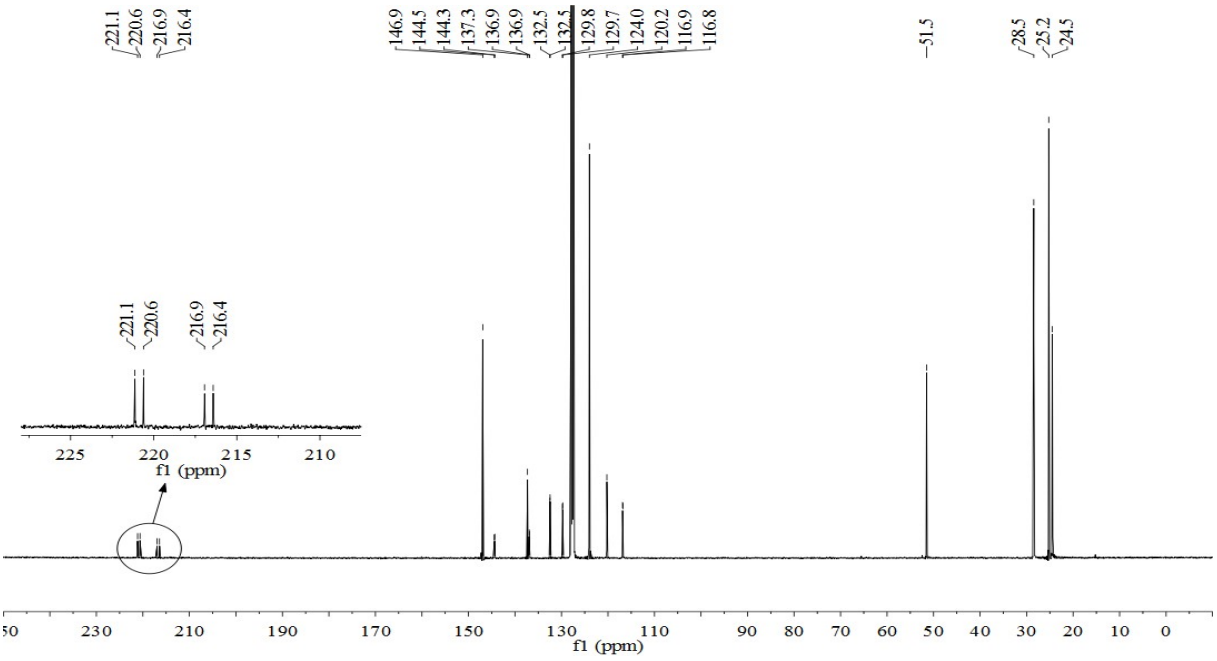



***Figure S10.*** $^{13}$C{$^{1}$H} NMR spectrum of **3** in $C_6D_6$.

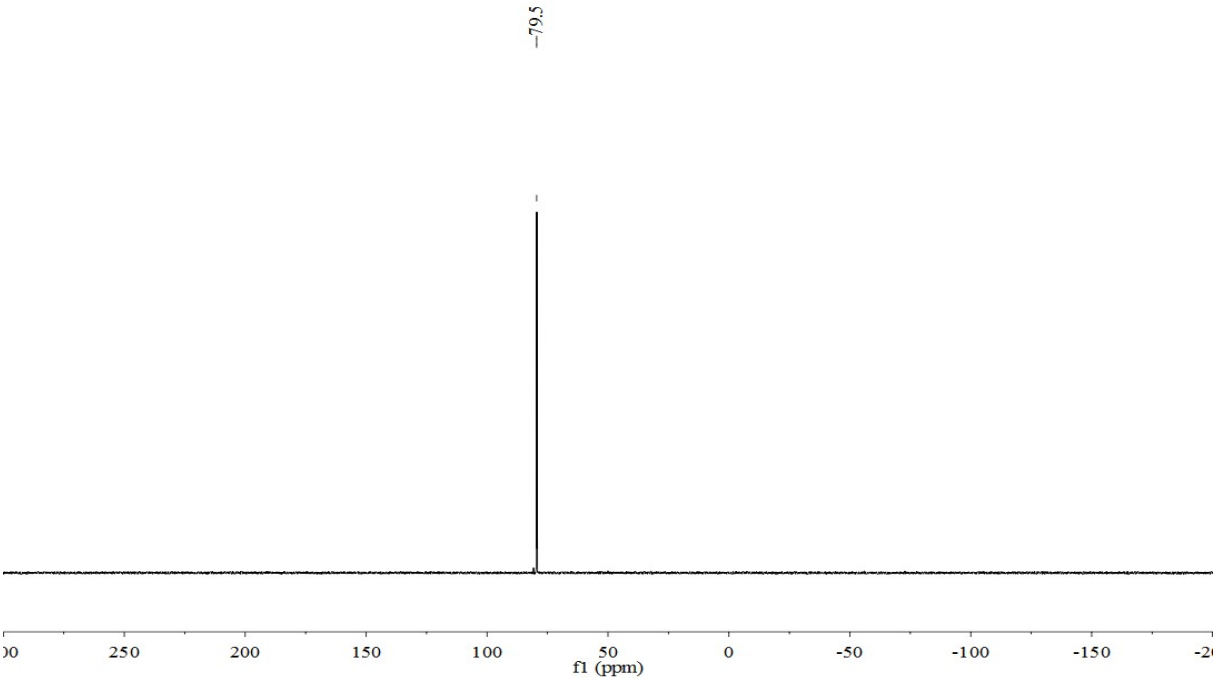



***Figure S11.*** $^{31}P\{^{1}H\}$ NMR spectrum of **3** in $C_6D_6$.

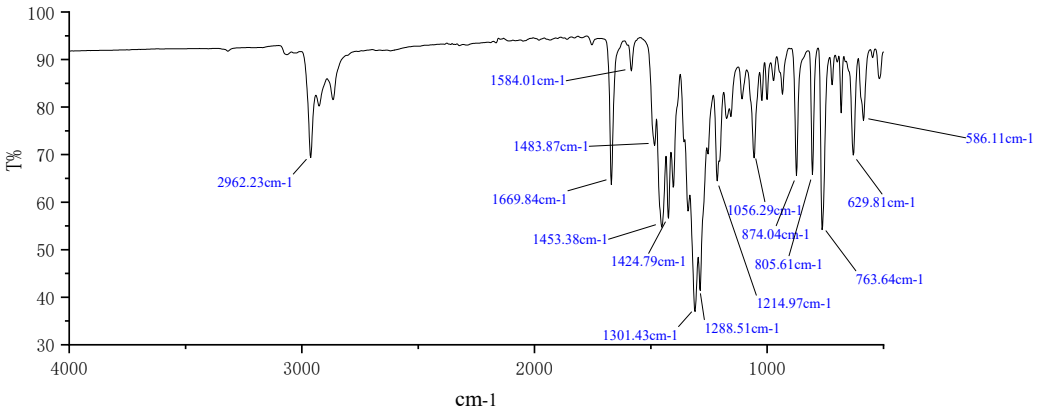
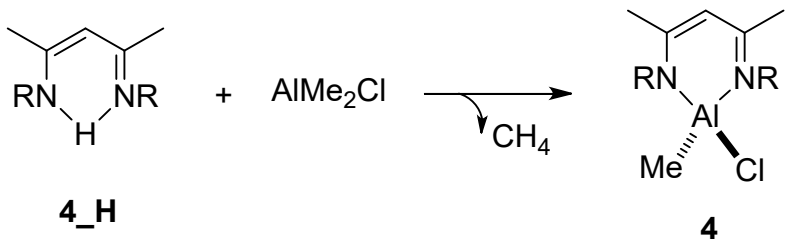



***Figure S12.*** IR spectrum of **3**




**4_H** **4**

**Preparation of 4:** A literature method was modified.[3] To a solution of **4_H** (4.19 g, 10 mmol) in toluene (20 mL) at 0 °C, $Me_2AlCl$ (11.1 mL, 0.9 M in heptane, 10 mmol) was added dropwise. After stirring for 1 hour at room temperature, the reaction mixture was stirred at 100 °C overnight. Then, the solvent was removed under reduced pressure and the remaining solid

was washed with hexane and dried *in vacuo* affording a white powder. This powder was redissolved in samll amount of diethyl ether and layered with hexane on top and stored at –30 °C. After 2 days, large amount of crystals were collected and dried *in vacuo* affording a white powder **4** (2.11 g, 4.26 mmol, 42.6 % yield). This material was used without further purification. M. P. = 187 °C. $^{1}$H NMR (400 MHz, $C_6D_6$): δ = 7.14 (m, 4H, $C_{ar}H$), 7.07 (m, 2H, $C_{ar}H$), 4.98 (s, 1H, γ-CH), 3.77 (m, 2H, C*H*$Me_2$), 3.21 (m, 2H, C*H*$Me_2$), 1.55 (s, 6H, $CH_3$), 1.46 (d, 6H, *J* = 6.4 Hz, $CH_3$), 1.28 (d, 6H, *J* = 6.8 Hz, $CH_3$), 1.19 (d, 6H, *J* = 6.8 Hz, $CH_3$), 1.01 (d, 6H, *J* = 6.8 Hz, $CH_3$), 0.64 (s, 3H, $CH_3$). $^{13}$C{H} NMR (100.5 MHz, $C_6D_6$): δ = 170.4 (s, *C*N), 145.7 (s, $C_{ar}$), 143.0 (s, $C_{ar}$), 139.4 (s, $C_{ar}$), 125.1 (s, $C_{ar}$), 123.7 (s, $C_{ar}$), 98.6 (γ-CH), 28.8 (s, $CH_3$), 27.8 (s, $CH_3$), 26.8 (s, $CH_3$), 24.6 (s, $CH_3$), 24.1 (s, $CH_3$), 23.6 (s, $CH_3$), 23.1(s, $CH_3$). Elemental analysis (%): calcd for $C_{30}H_{44}N_2ClAl$; C 72.76, H 8.96; found: C 71.52, H 9.33.

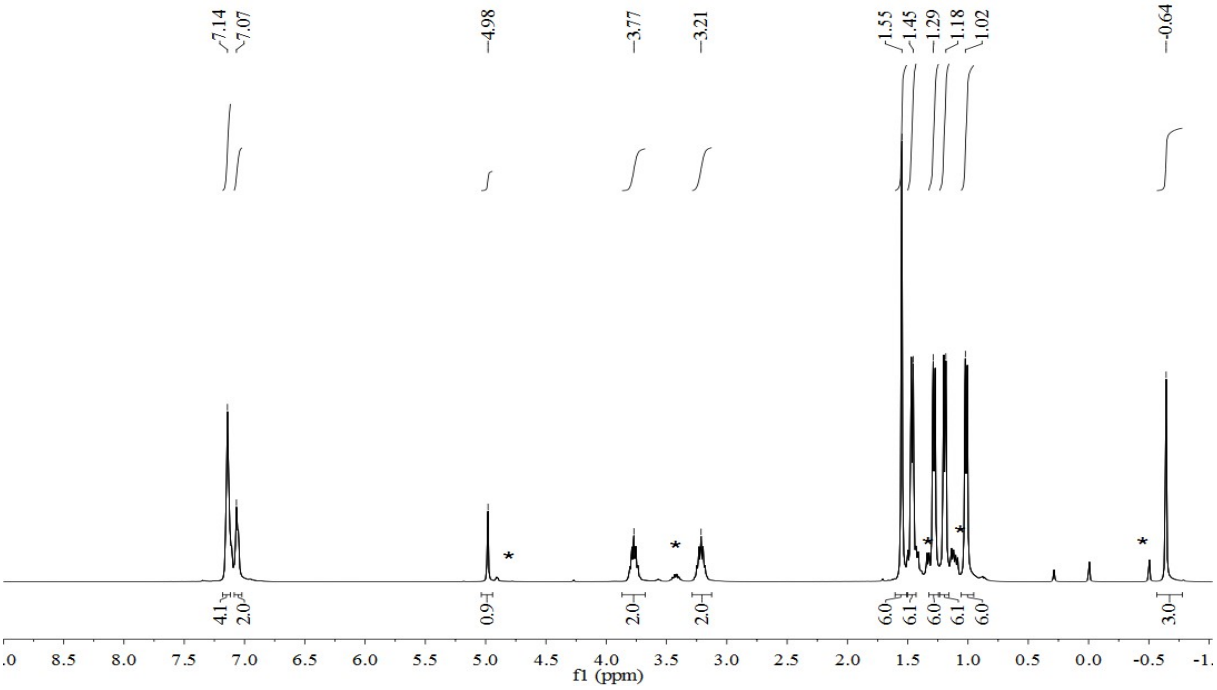



***Figure S13.*** $^{1}$H NMR spectrum of **4** in $C_6D_6$. *Small amount of impurity.

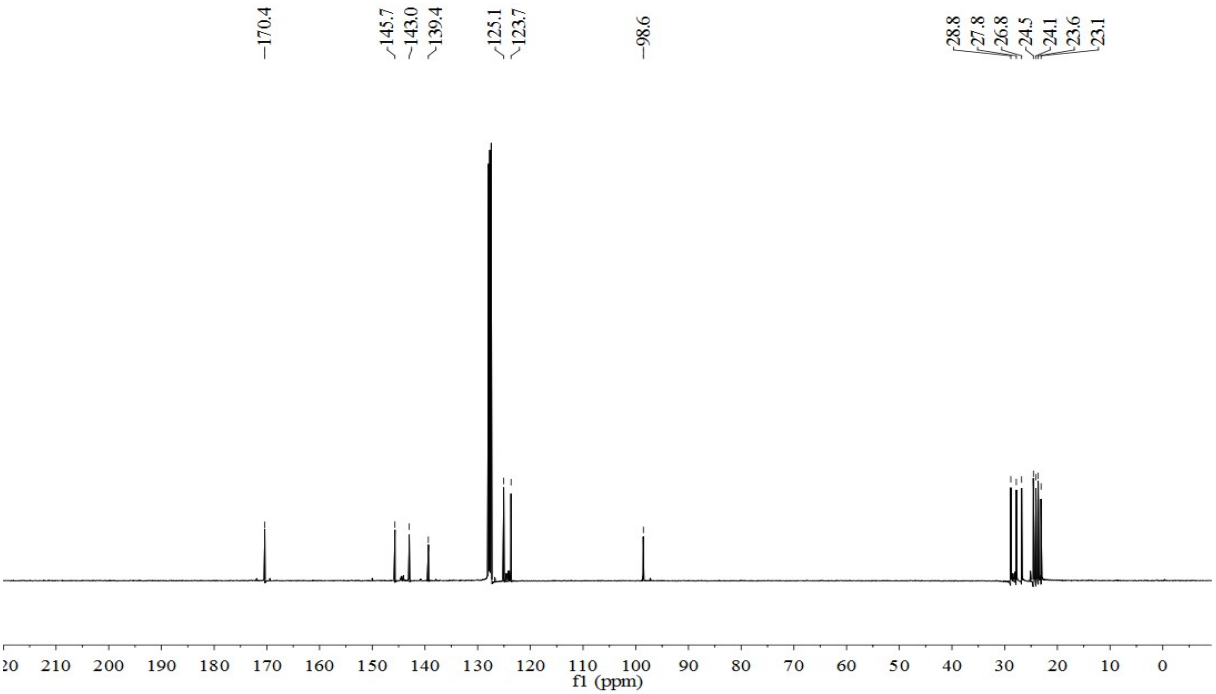
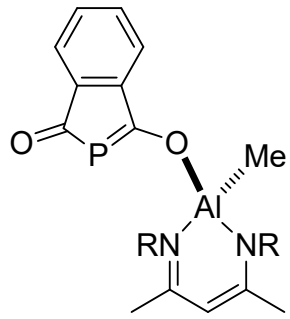



***Figure S14.*** $^{13}C\{^{1}H\}$ NMR spectrum of **4** in $C_6D_6$.




**5**

**Preparation of 5: 4** (247.0 mg, 0.5 mmol) in THF (4 mL) was added dropwise to a stirred solution of **1** (1.2 equivalent) in THF (4 mL). After stirring for 1 hour, the solvent was removed under reduced pressure. The remaining residue was extracted with diethyl ether, then the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* affording a red powder **5** (286.3 mg, 0.46 mmol, 92.0 % yield). Red crystals of **5** were obtained from the saturated diethyl ether and hexane solution via slow evoporateion. M. P. = 216 °C. $^{1}H$ NMR (400 MHz, $C_6D_6$): δ = 7.53 (d, 1H, *J* = 6.8 Hz, $C_{ar}H$), 7.20 (d, 1H, *J* = 7.2 Hz, $C_{ar}H$), 7.10 (m, 2H, $C_{ar}H$), 7.05 (m, 2H, $C_{ar}H$), 7.00 (m, 2H, $C_{ar}H$), 6.84 (m, 2H, $C_{ar}H$), 5.20 (s, 1H, γ-CH), 3.35 (m, 4H, $CHMe_2$), 3.17 (m, 4H, $CH_2$), 1.51 (s, 6H, $CH_3$), 1.29 (d, 6H, *J* = 6.8 Hz, $CH_3$), 0.97 (m, 18H, $CH_3$), –0.64 (s, 3H, Al-$CH_3$). $^{13}C\{H\}$ NMR (100.5 MHz, $C_6D_6$): δ = 231.9 (d, $J_{CP}$ = 57.5 Hz, *C*OPCOAl), 221.9 (d, $J_{CP}$ = 55.2 Hz, COP*C*OAl), 171.0 (s, $C_{ar}$),

146.8 (d, $J_{CP}$ = 9.0 Hz, $C_{ar}$), 145.4 (s, $C_{ar}$), 143.0 (s, $C_{ar}$), 139.2 (s, $C_{ar}$), 132.3 (s, $C_{ar}$), 129.9 (s, $C_{ar}$), 124.6 (s, $C_{ar}$), 123.8 (s, $C_{ar}$), 119.2 (s, $C_{ar}$), 117.0 (d, $J_{CP}$ = 8.6 Hz, $C_{ar}$), 100.7 (d, $J_{CP}$ = 6.1 Hz, $C_{ar}$), 28.8, 28.3 (d, $J_{CP}$ = 3.6 Hz, POAlMe), 25.7, 24.4, 23.9, 23.7, 22.9. $^{31}P\{H\}$ NMR (161.9 MHz, $C_6D_6$): δ = 77.6 (s). Elemental analysis (%): calcd for $C_{38}H_{48}N_2O_2PAl$; C 73.27, H 7.77; found: C 73.38, H 7.89. **IR** (ATR, [$cm^{-1}$]): 1650.5 (C=O).

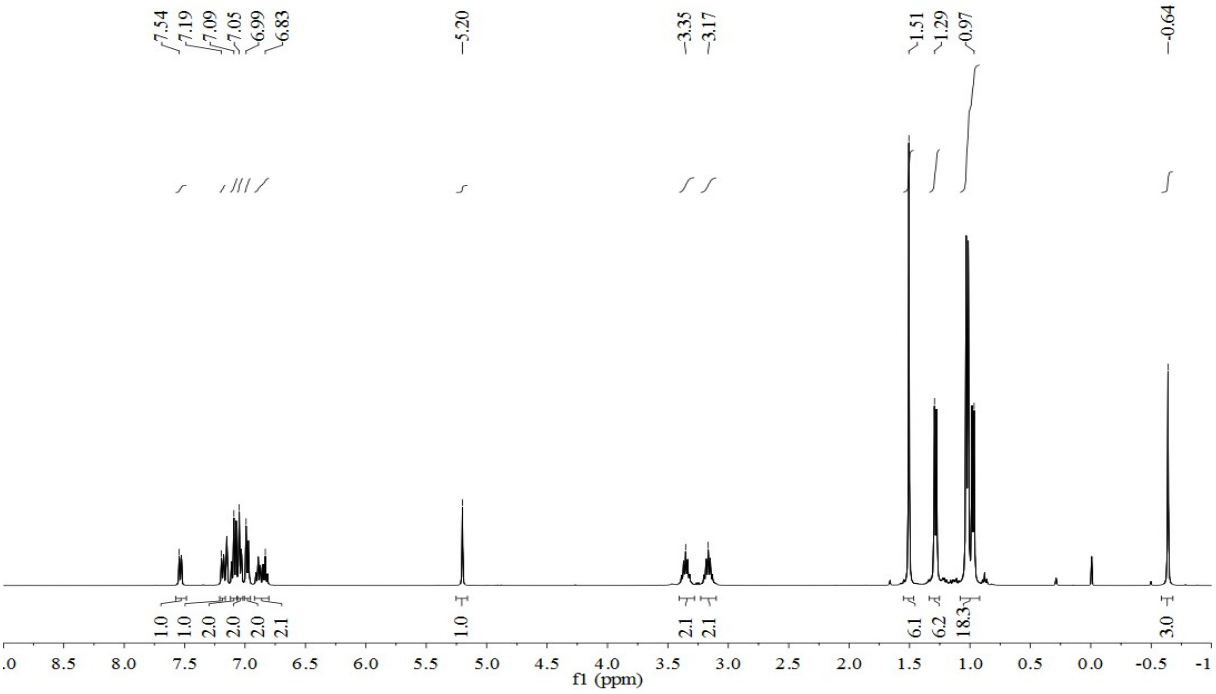



***Figure S15.*** $^{1}H$ NMR spectrum of **5** in $C_6D_6$.

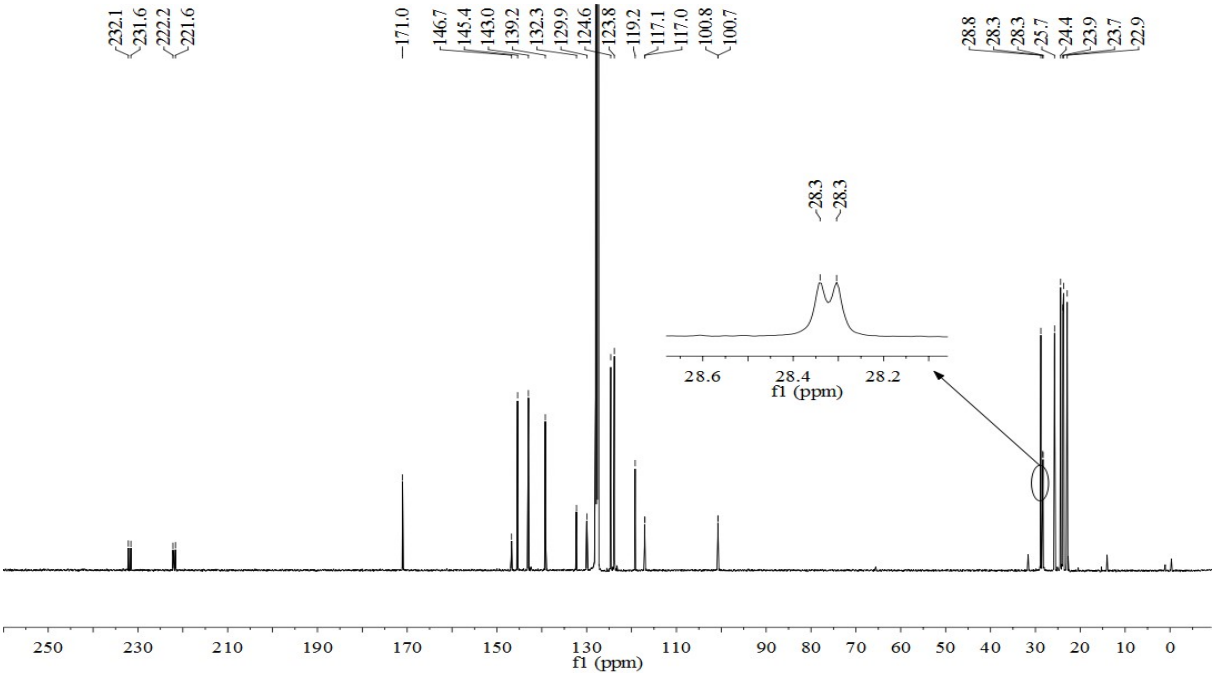


***Figure S16.*** $^{13}C\{^{1}H\}$ NMR spectrum of **5** in $C_6D_6$.

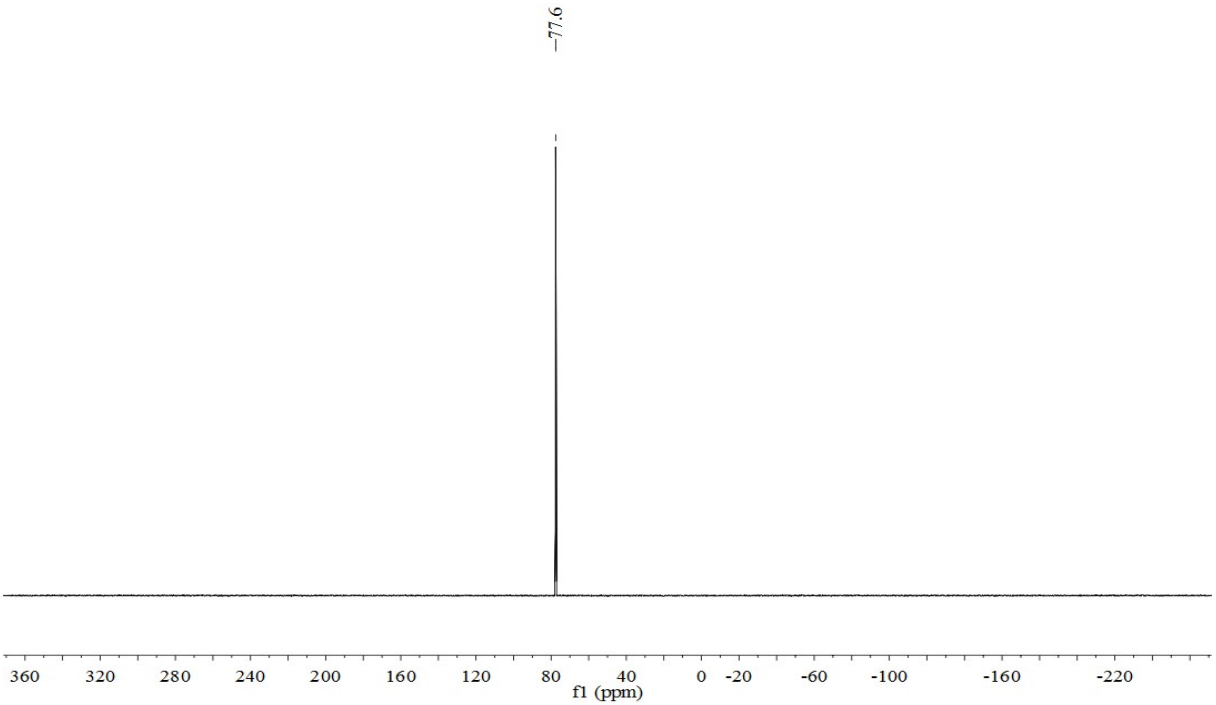



***Figure S17.*** $^{31}P\{^{1}H\}$ NMR spectrum of **5** in $C_6D_6$.

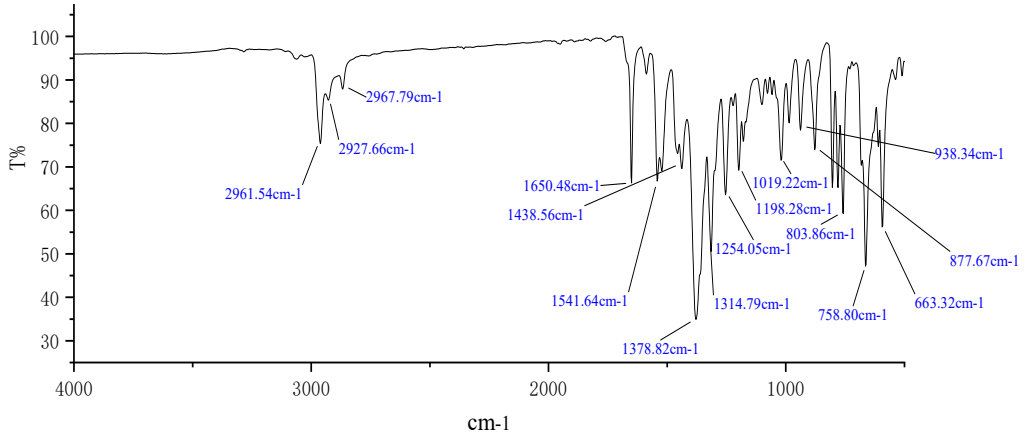
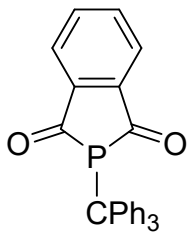



***Figure S18.*** IR spectrum of **5**




**6**

**Preparation of Triphenylmethyl-isophosphindoline-1,3-dione** (**6**): Triphenylmethyl chloride ($Ph_3CCl$, 140 mg, 0.5 mmol) was added dropwise to a stirred solution of **1** (1.2 equivalent) in THF (20 mL). After stirring for 24 hours, the solvent was removed under reduced pressure. The remaining residue was extracted with dichloromethane, then the solvent was removed under reduced pressure. The remaining solid was dried *in vacuo* affording a yellow powder **6** (890 mg, 2.19 mmol, 54.8 % yield). $^{1}$H NMR (300 MHz, D$^6$-DMSO): δ = 7.89 (m, 2H, $C_{ar}H$), 7.72 (m, 2H, $C_{ar}H$), 7.29 (m, 15H, $C_{ar}H$). $^{13}$C{H} NMR (75.5 MHz, D$^6$-DMSO): δ = 211.0 (d, $J_{CP}$ = 34.9 Hz, *C*O), 143.60 (d, $J_{CP}$ = 5.62 Hz, $C_{ar}$), 142.23 (d, $J_{CP}$ = 18.07 Hz, $C_{ar}$), 136.63 (s, $C_{ar}$), 129.66 (d, $J_{CP}$ = 8.43 Hz, $C_{ar}$), 128.67 (s, $C_{ar}$), 127.46 (s, $C_{ar}$), 122.70 (s, $C_{ar}$), 64.69 (d, $J_{CP}$ = 20.48 Hz). $^{31}$P{H} NMR (161.9 MHz, D$^6$-DMSO): δ = 9.01 (s). Elemental analysis (%): calcd for $C_{27}H_{19}O_2P$; C 79.79, H 4.71; found: C 79.91, H 4.58.**IR** (ATR, [cm$^{-1}$]): 1663.3, 1649.3 (C=O).

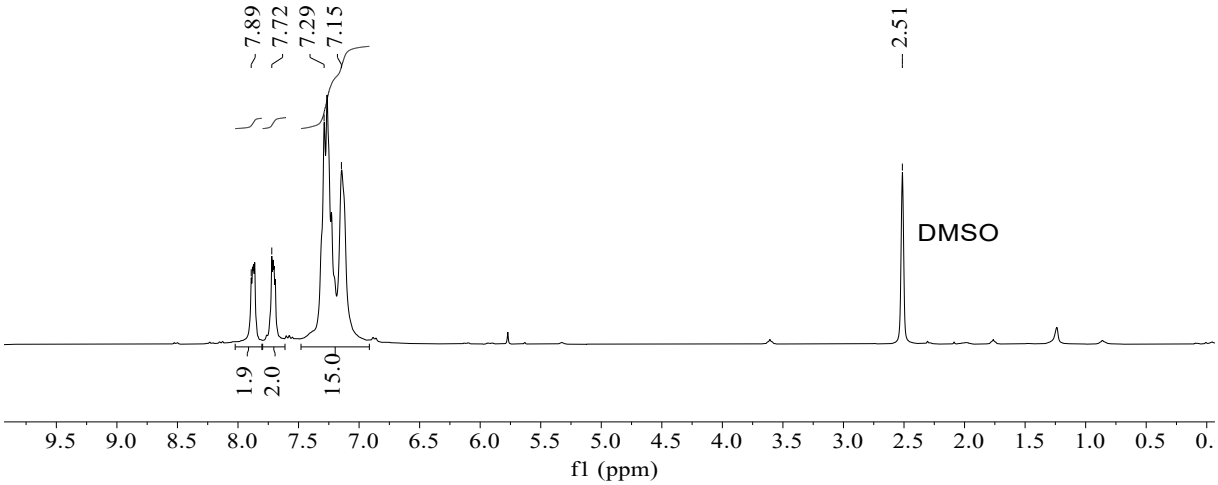



***Figure S19.*** $^{1}$H NMR spectrum of **6** in D$^6$-DMSO.

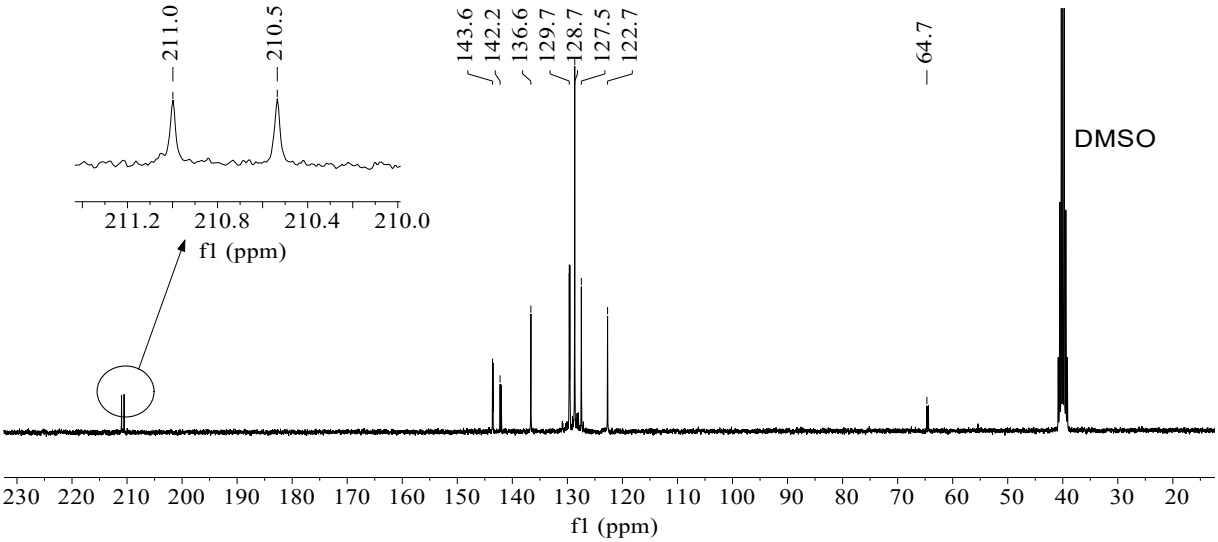



***Figure S20.*** $^{13}$C{$^{1}$H} NMR spectrum of **6** in D$^6$-DMSO.

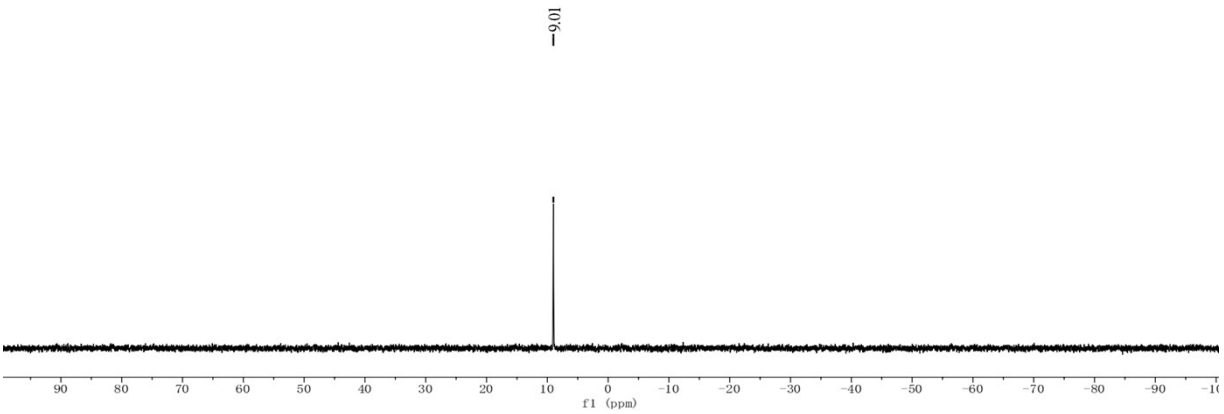



***Figure S21.*** $^{31}P\{^{1}H\}$ NMR spectrum of **6** in $D^{6}$-DMSO.

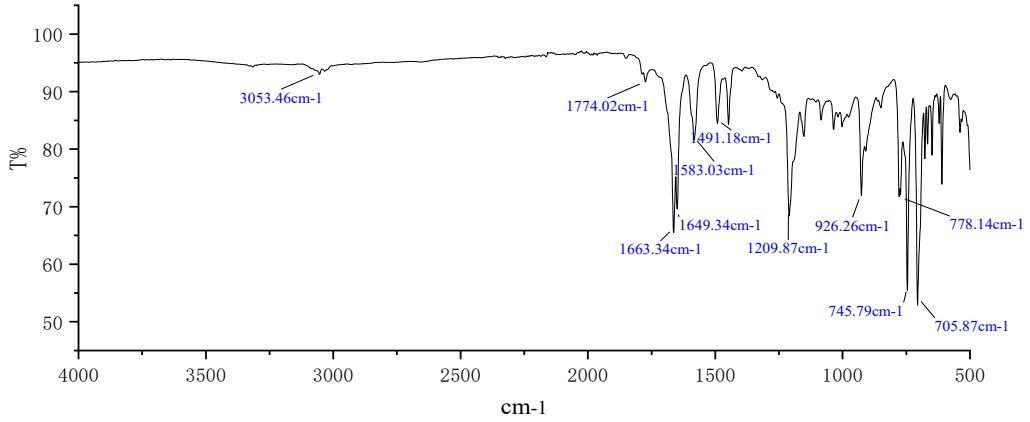
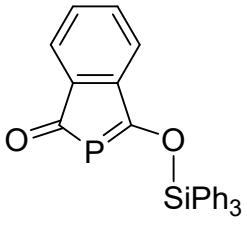



***Figure S22.*** IR spectrum of **6**




**7**

**Preparation of 3-triphenylsilyloxy-1*H*-isophosphindol-1-one** (**7**): $Ph_3SiCl$ (29.5 mg, 0.01 mmol) in THF (1 mL) was added dropwise to a stirred solution of **1** (1.0 equivalent) in THF (1 mL). After stirring for 2 minutes, the $^{31}P$ NMR spectrum indicates the formation of **7** at 82.3 ppm. However, this compound decomposes with time and thus pure form cannot be obtained.

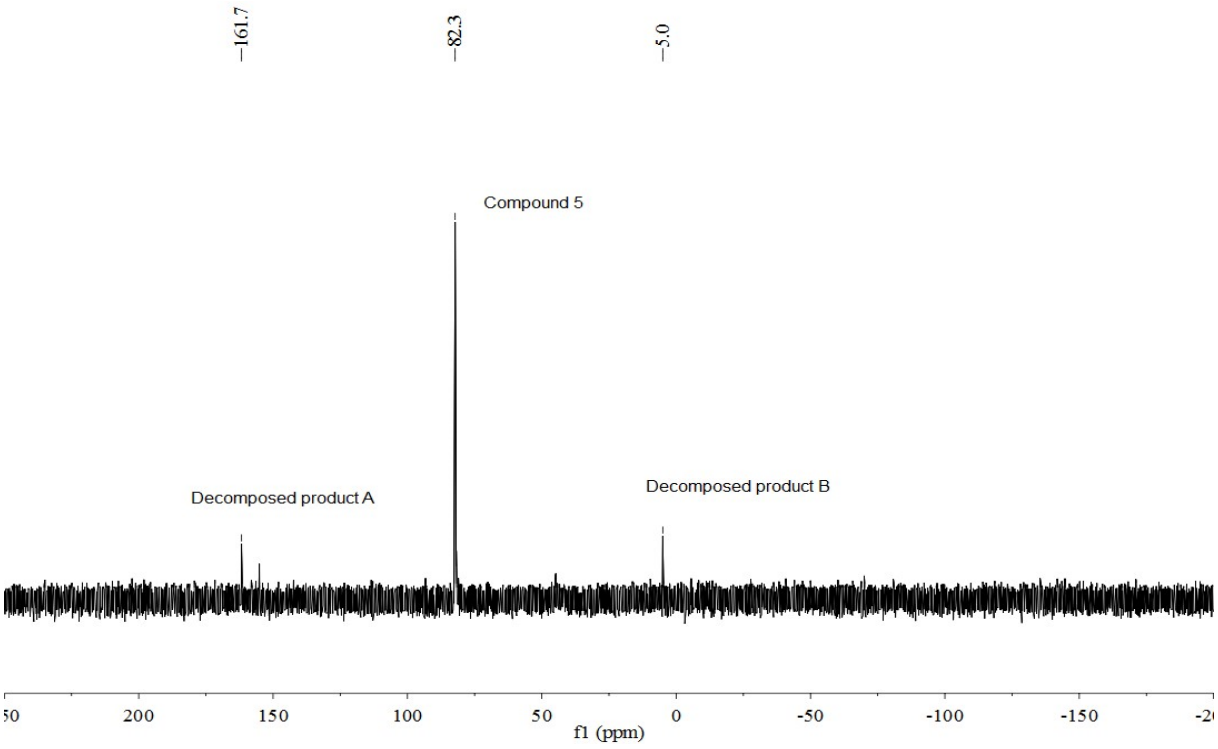
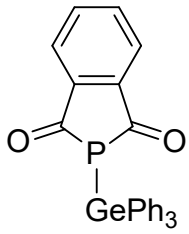



***Figure S23.*** $^{31}P\{^{1}H\}$ NMR spectrum of reaction mixture in THF.




**8**

**Preparation of 2-triphenylgermyl-isophosphindoline-1,3-dione** (**8**): $Ph_3GeCl$ (169.7 mg, 0.5 mmol) in THF (2 mL) was added dropwise to a stirred solution of **1** (1.2 equivalent) in THF (4 mL). After stirring for 1 hours, the solvent was removed under reduced pressure. The remaining residue was extracted with dichloromethane, then the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* affording a yellow powder **8** (202.7 mg, 0.43 mmol, 86.8 % yield). Yellow crystals of **8** were obtained from a fluorobenzene solution layered with hexane on top and stored at –30 °C. M. P. = 122 °C. $^{1}H$ NMR (400 MHz, $CDCl_3$): δ = 7.58 (m, 4H, $C_{ar}H$), 7.47 (m, 6H, $C_{ar}H$), 7.33 (m, 9H, $C_{ar}H$). $^{13}C\{H\}$ NMR (100.5 MHz, $CDCl_3$): δ = 215.5 (d, $J_{CP}$ = 38.4 Hz, *C*O), 143.7 (d, $J_{CP}$ = 11.8 Hz, $C_{ar}$), 135.0 (s, $C_{ar}$), 134.2 (s, $C_{ar}$), 133.2 (d, $J_{CP}$ = 7.2 Hz, $C_{ar}$), 129.9 (s, $C_{ar}$), 121.3 (s, $C_{ar}$). $^{31}P\{H\}$ NMR (161.9 MHz, $CDCl_3$): δ = –70.6 (s). Elemental analysis (%): calcd for

$C_{26}H_{19}O_2PGe$; C 66.84, H 4.10; found: C 66.96, H 4.01. **IR** (ATR, [$cm^{-1}$]): 1658.8, 1642.8 (C=O), 1643 (C=O).

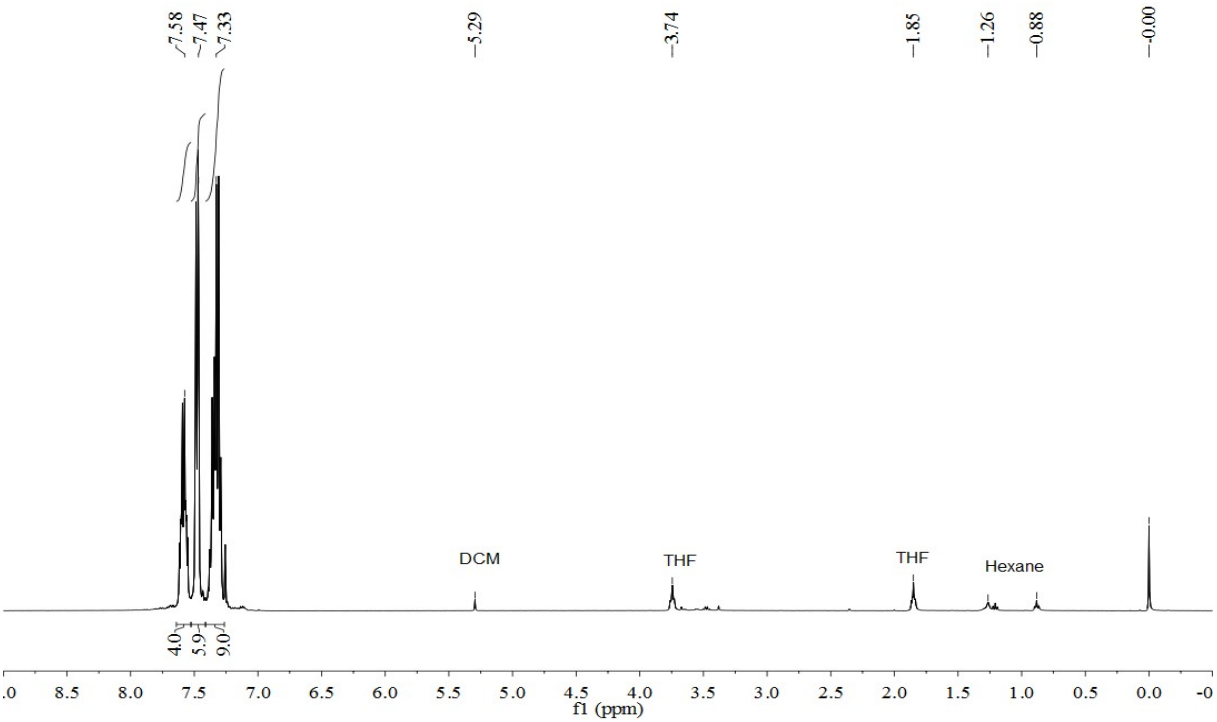



***Figure S24.*** $^{1}H$ NMR spectrum of **8** in $CDCl_3$.

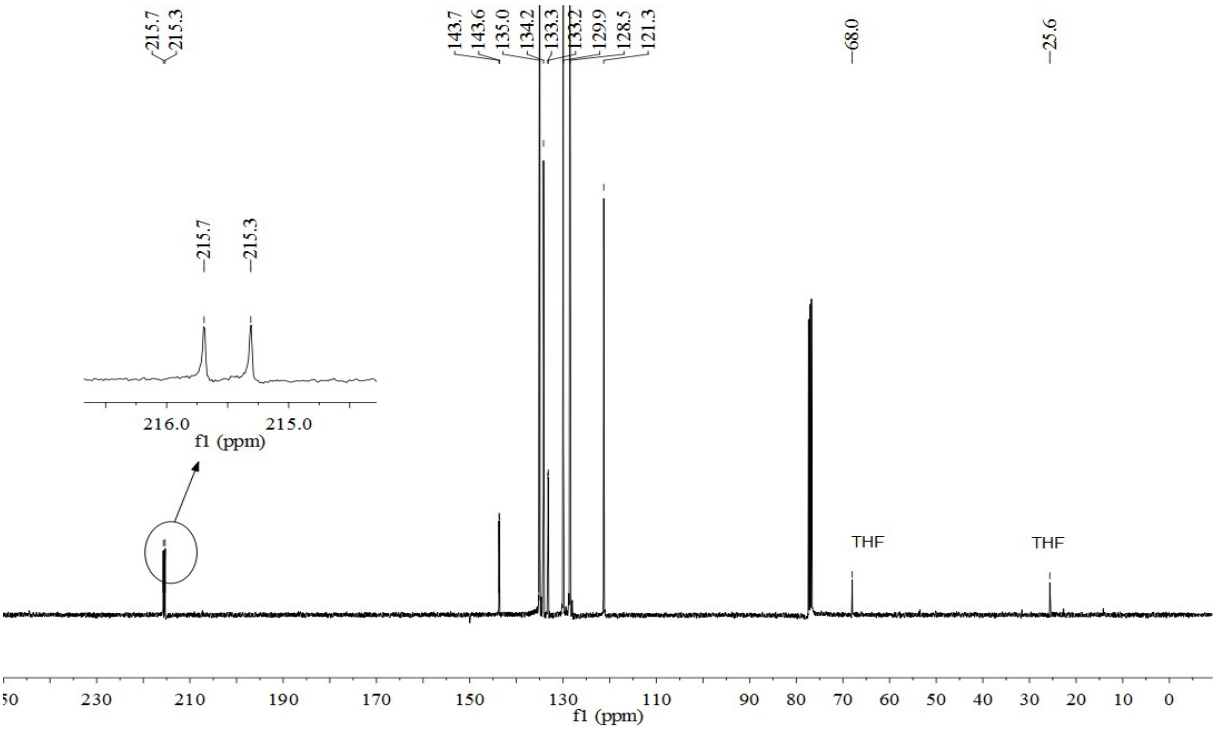



***Figure S25.*** $^{13}C\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$.

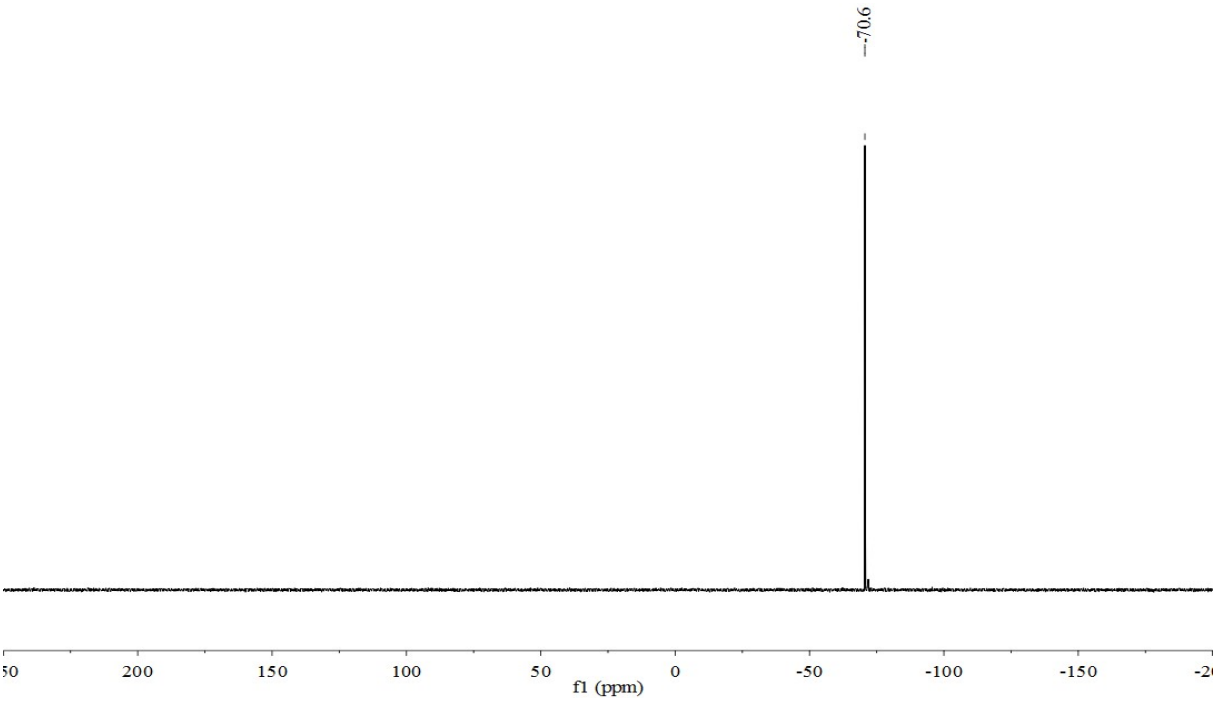



***Figure S26.*** $^{31}P\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$.

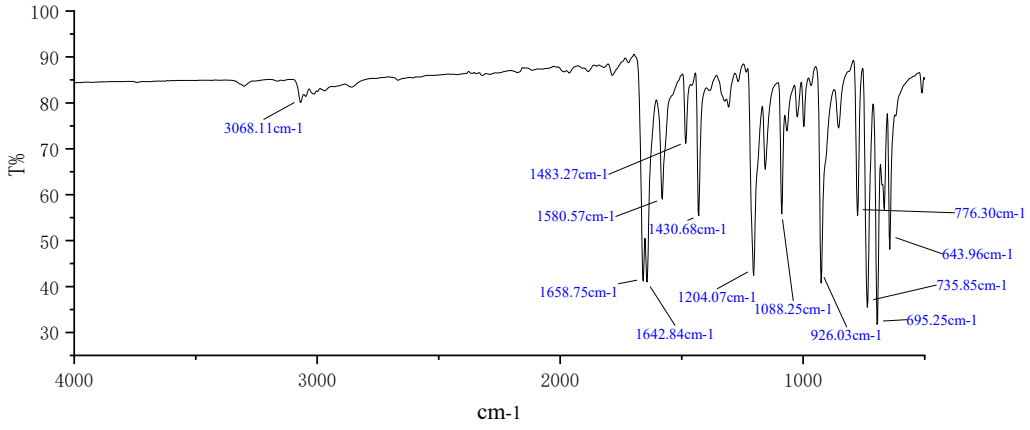
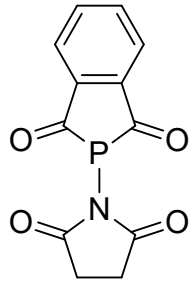



***Figure S27.*** IR spectrum of **8**




**9**

**Preparation of 9**: N-Bromosuccinimide (66.8 mg, 0.5 mmol) in toluene (6 mL) was added dropwise to a stirred solution of **1** (1.2 equivalent) in toluene (4 mL) at –80 °C. After stirring for 1 hours at room temperature, all precipitates were filtered off. Then the filtrate was concentrated, and the remaining solid was washed with hexane and dried *in vacuo* affording a yellow powder **9** and **10** as mixture. Yellow crystals were obtained from a toluenesolution of the mixture layered with hexane on top and stored at –30 °C. After checked by the single crstal X-ray diffraction, two kinds of crystals were found, one was proved to be compound **9**, the other was **10**. $^{31}P\{H\}$ NMR (161.9 MHz, toluene): δ = –35.8 (s). The signal at –58.4 ppm in toluene presumbly belongs to **10**, which is 58.4 ppm in $CDCl_3$.

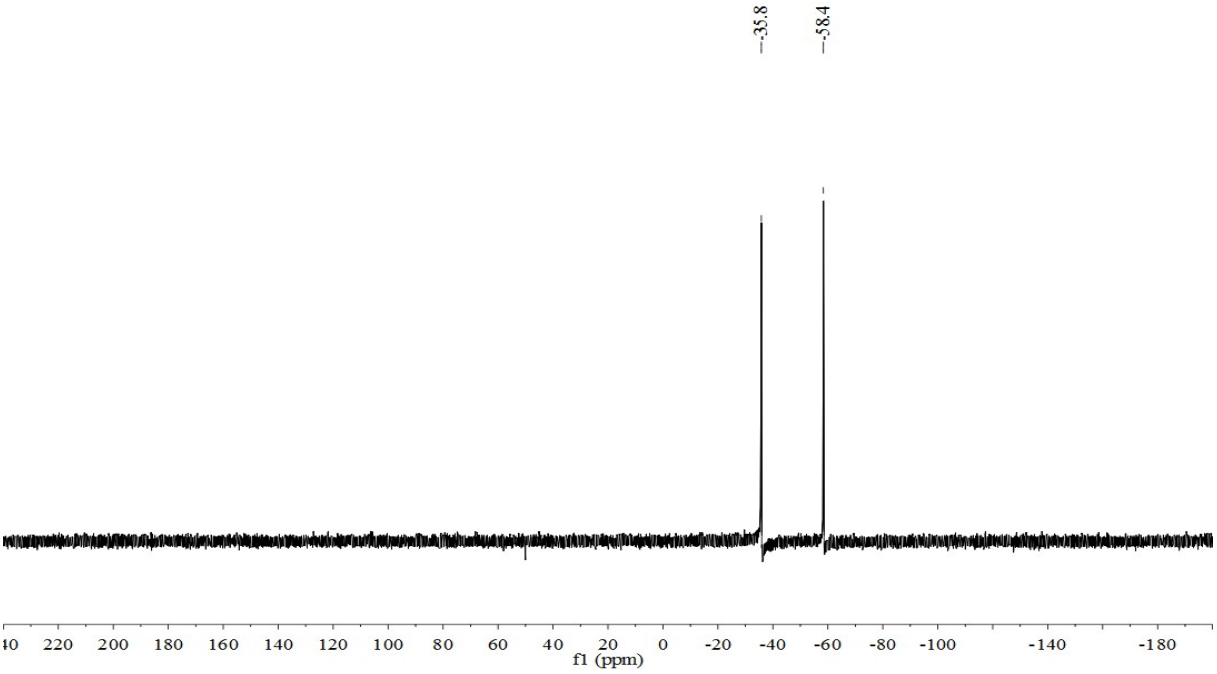
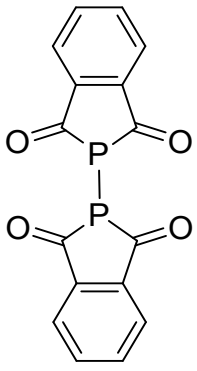



***Figure S28.*** $^{31}P\{^{1}H\}$ NMR spectrum of **9** and **10** in toluene.



**10**

**Synthesis of 2,2'-biisophosphindole-1,1',3,3'-tetraone** (**10**): Iodine (63.5 mg, 0.5 equiv.) in toluene (2 ml) was added dropwise to a toluene (5 ml) solution of **1** (1.2 equivalent). After stirring for 1 hours, the solvent was removed under reduced pressure. The remaining residue was extracted with diethyl ether, then the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* affording a yellow powder **10** (126.1 mg, 0.39 mmol, 77.3 % yield). Yellow crystals of **10** were obtained from a saturated solution of diethyl ether and hexane via slow evaporation. M.P. = 157 °C. $^{1}$H NMR (400 MHz, $CDCl_3$): δ = 7.93 (m, 4H, $C_{ar}H$), 7.87(m, 4H, $C_{ar}H$). $^{13}$C{H} NMR (100.5 MHz, $CDCl_3$): δ = 208.9 (virtual triplet, *C*OP), 143.1 (virtual triplet, $C_{ar}$), 135.9 (s, $C_{ar}$), 122.8 (s, $C_{ar}$). $^{31}$P{H} NMR (161.9 MHz, $CDCl_3$): δ = –56.5 (s). Elemental analysis (%): calcd for $C_{16}H_8O_4P_2$; C 58.90, H 2.47; found: C 58.55, H 2.73. **IR** (ATR, [$cm^{-1}$]): 1778.5, 1755.5, 1718.1, 1662.6 (C=O).

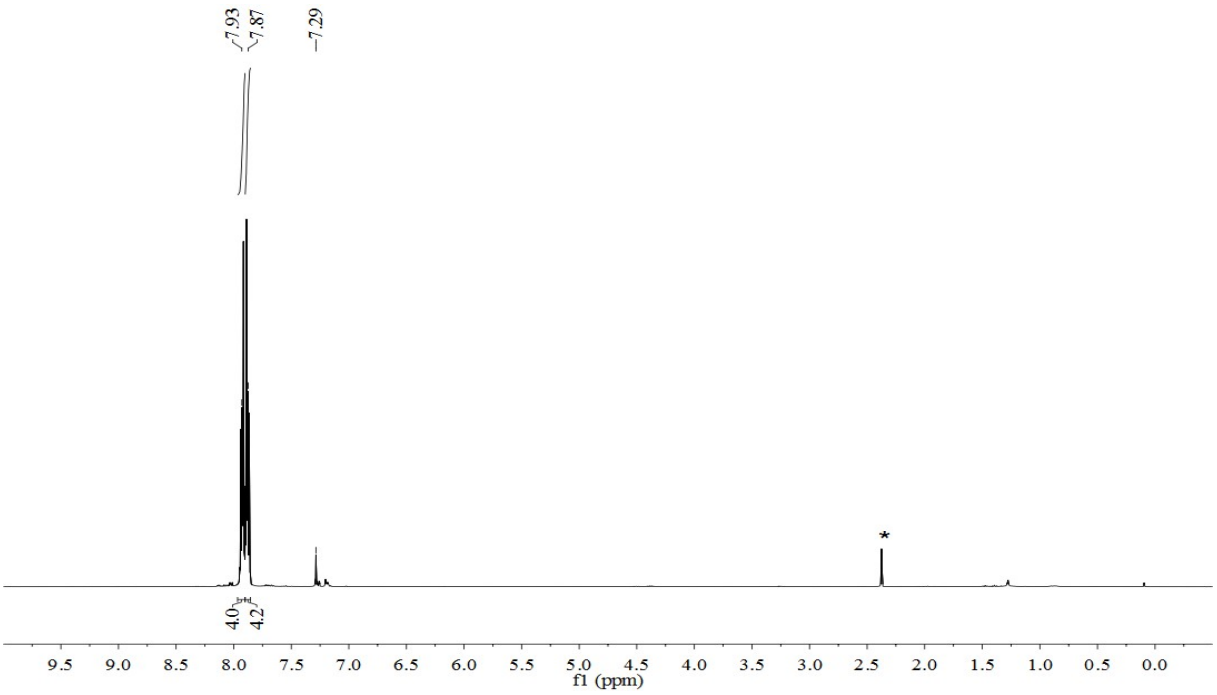



***Figure S29.*** $^{1}$H NMR spectrum of **10** in $CDCl_3$. *Toluene.

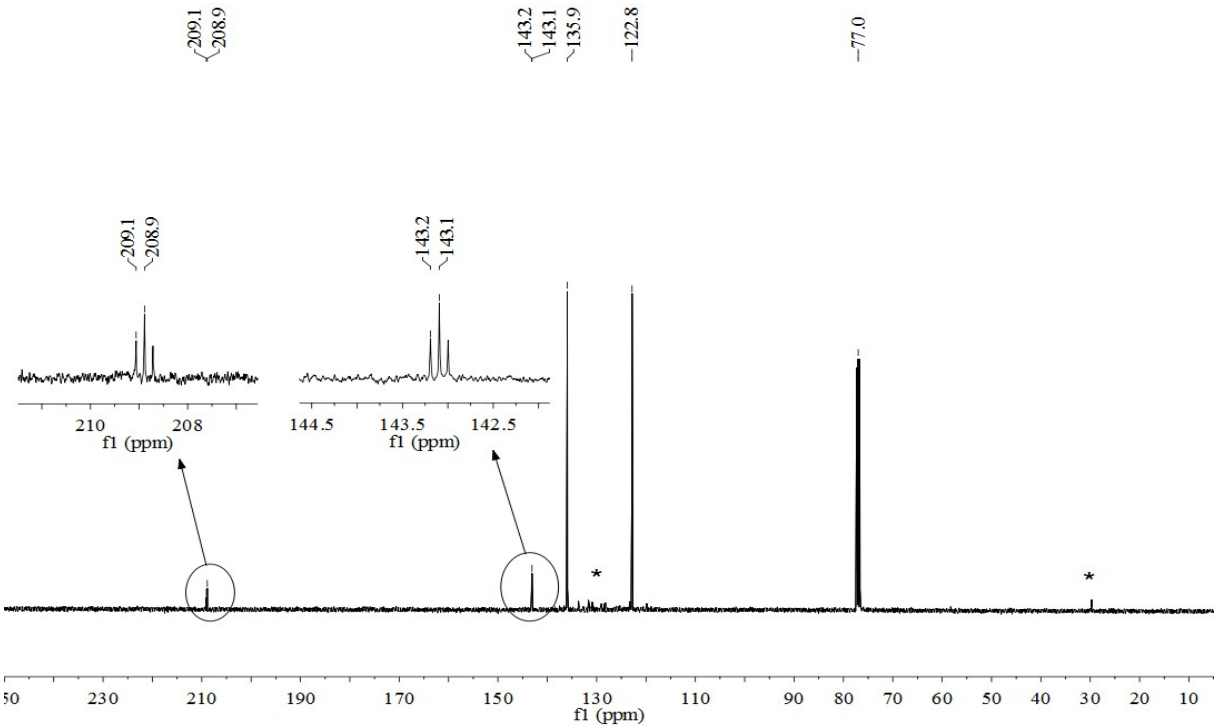



***Figure S30.*** $^{13}C\{^{1}H\}$ NMR spectrum of **10** in $CDCl_3$. *Toluene.

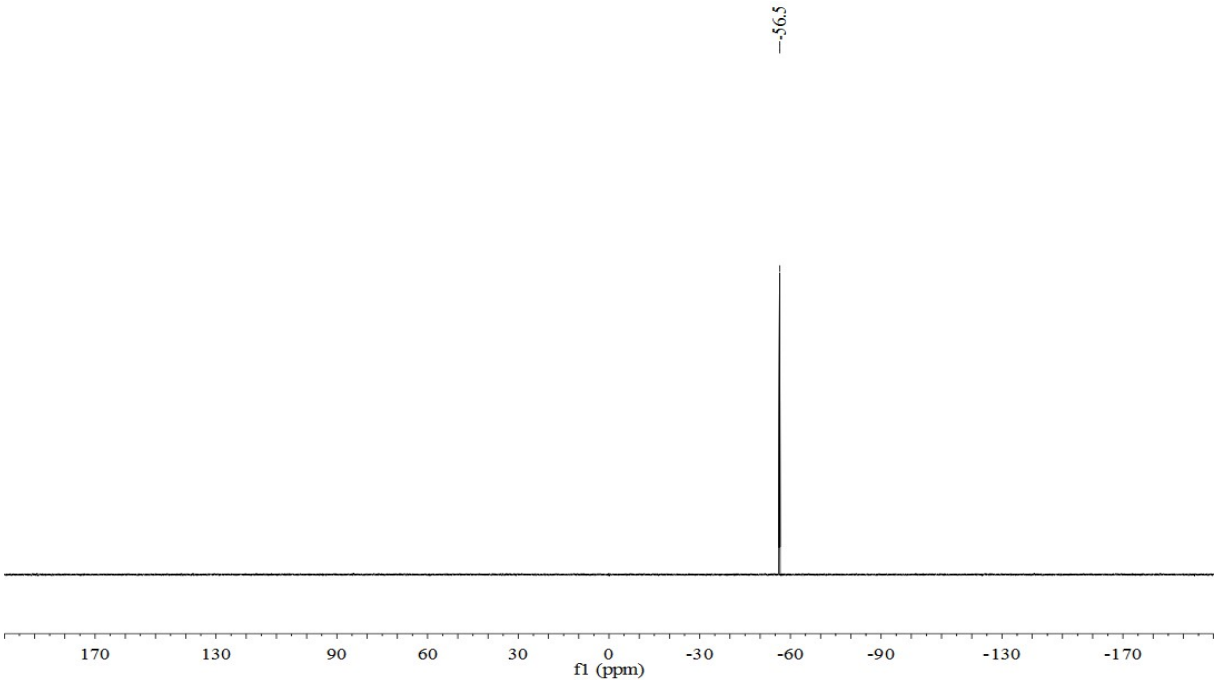



***Figure S31.*** $^{31}P\{^{1}H\}$ NMR spectrum of **10** in $CDCl_3$.

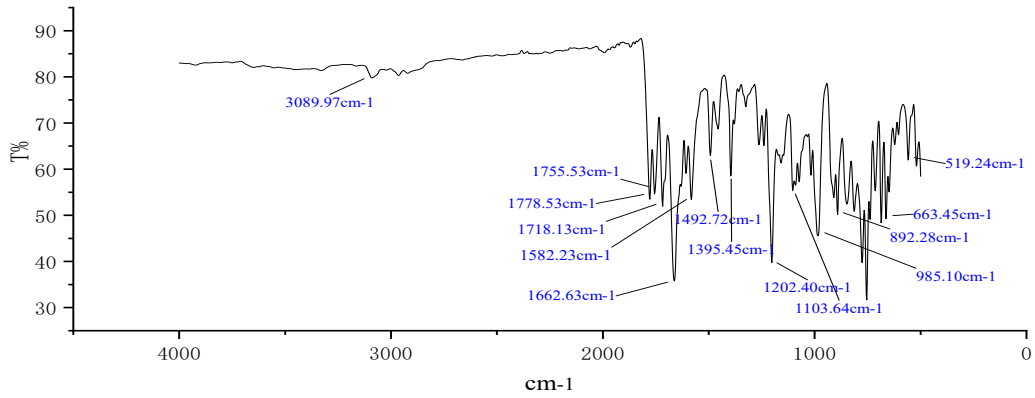
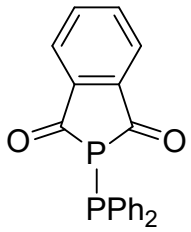



***Figure S32.*** IR spectrum of **10**




**11**

**Preparation of 2-diphenylphosphino-isophosphindoline-1,3-dione** (**11**): $Ph_2PCl$ (110.3 mg, 0.5 mmol) in THF (2 mL) was added dropwise to a stirred solution of **1** (1.2 equivalent) in THF (4 mL). After stirring for 1 hours, the solvent was removed under reduced pressure. The remaining residue was extracted with dichloromethane, then the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* affording a yellow powder **11** (155.3 mg, 0.45 mmol, 89.2 % yield). Yellow crystals of **11** were obtained from a fluorobenzene solution layered with hexane on top and stored at –30 °C. M. P. = 111 °C. $^{1}$H NMR (400 MHz, $CDCl_3$): δ = 7.71 (m, 4H, $C_{ar}H$), 7.49 (m, 4H, $C_{ar}H$), 7.29 (m, 6H, $C_{ar}H$). $^{13}$C{H} NMR (100.5 MHz, $CDCl_3$): δ = 212.7 (dd, $^{1}J_{CP}$ = 36.6 Hz, $^{2}J_{CP}$ = 7.4 Hz, *C*O), 143.1 (d, $J_{CP}$ = 14.3 Hz, $C_{ar}$), 135.0 (s, $C_{ar}$), 134.1 (dd, $J_{CP}$ = 20.8 Hz, $J_{CP}$ = 6.5 Hz, $C_{ar}$), 132.4 (dd, $^{1}J_{CP}$ = 22.0 Hz, $^{2}J_{CP}$ = 3.4 Hz,), 129.6 (s, $C_{ar}$), 128.6 (d, $J_{CP}$ = 7.1 Hz, $C_{ar}$). $^{31}$P{H} NMR (161.9 MHz, $CDCl_3$): δ = –0.9 (d, $J_{PP}$ = 73.5 Hz, P*P*$Ph_2$), –38.9 (d, $J_{PP}$ = 73.5 Hz, *P*P$Ph_2$) . Elemental analysis (%): calcd for $C_{20}H_{14}O_2P_2$; C 68.96, H 4.05; found: C 69.17, H 4.26. **IR** (ATR, [$cm^{-1}$]): 1662.2, 1649.5 (C=O).

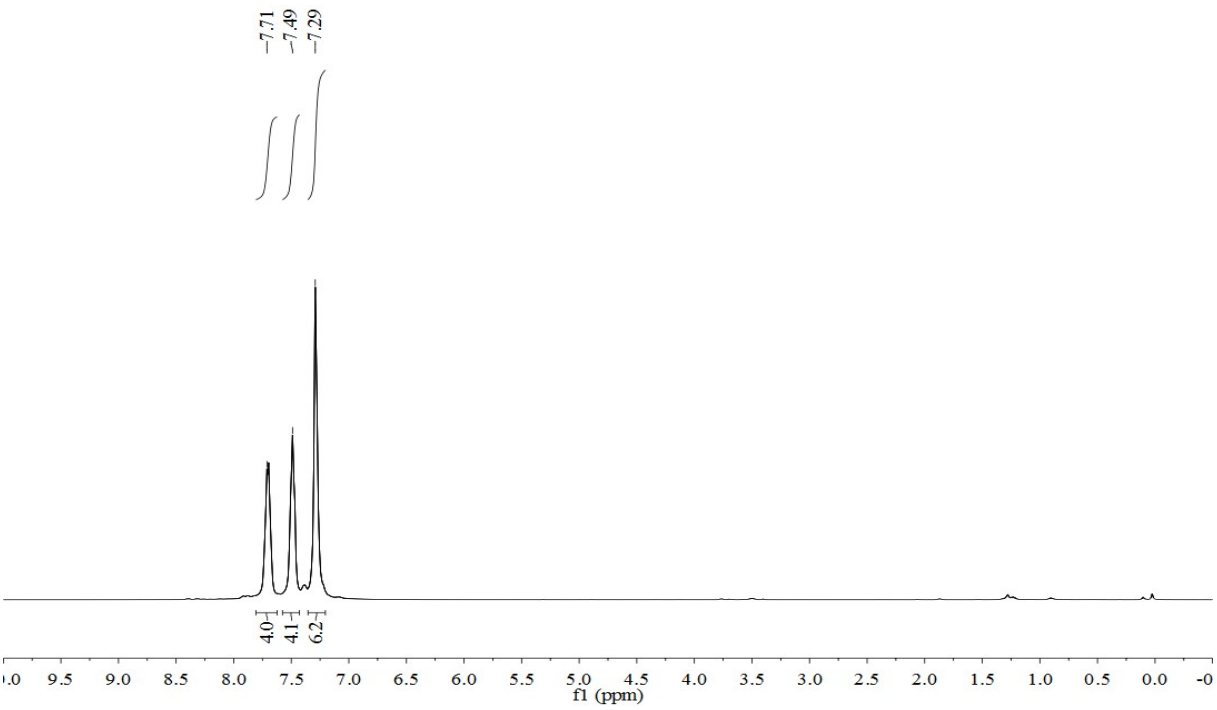



***Figure S33.*** $^{1}H$ NMR spectrum of **11** in $CDCl_3$.

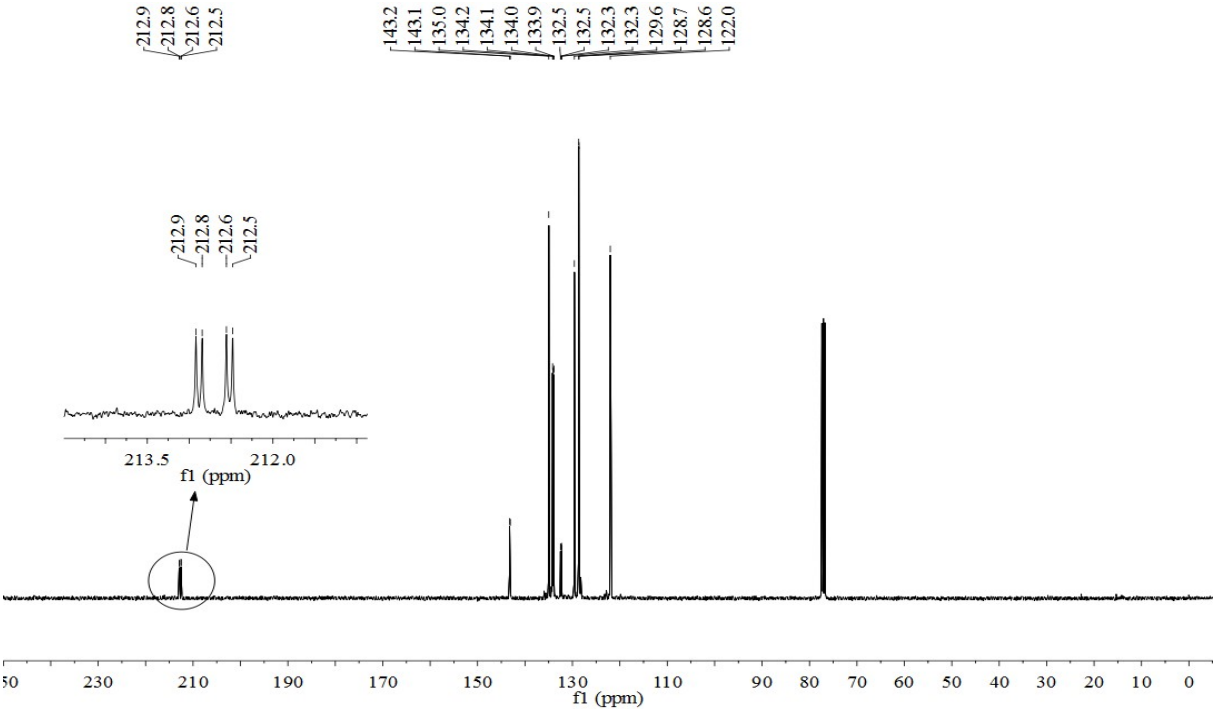



***Figure S34.*** $^{13}C\{^{1}H\}$ NMR spectrum of **11** in $CDCl_3$.

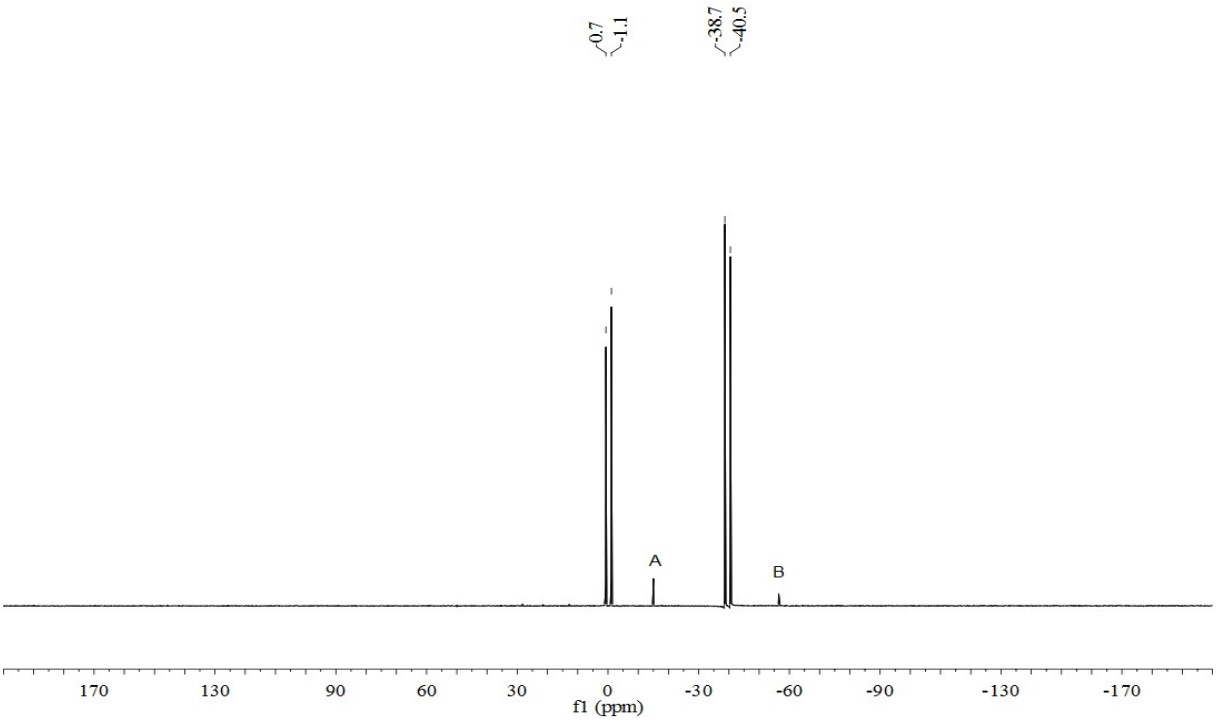



***Figure S35.*** $^{31}P\{^{1}H\}$ NMR spectrum of **11** in $CDCl_3$. A and B are samll impurities.

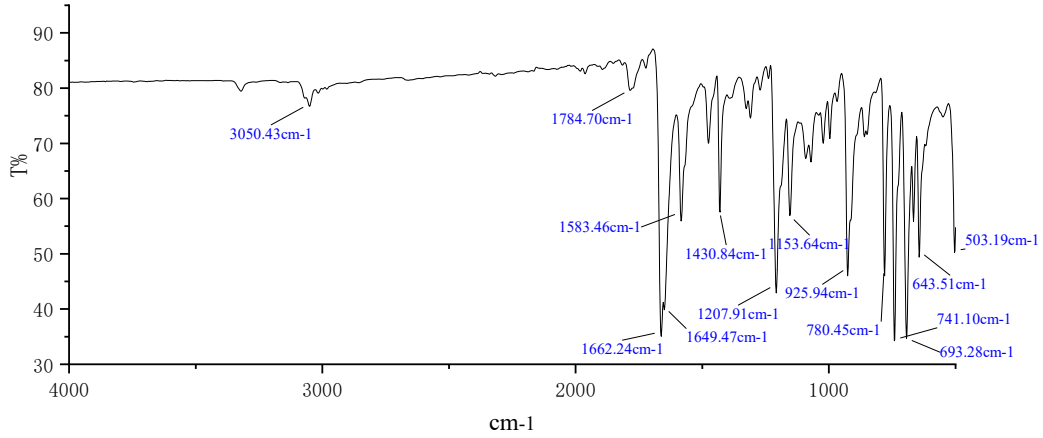



***Figure S36.*** IR spectrum of **11**

**Preparation of 13**: **12** (222.5 mg, 0.5 equiv.) in THF (2 ml) was added dropwise to a stirred solution of **1** (1.2 equivalent) in THF (4 mL). After stirring for 2 hours, the solvent was removed under reduced pressure. The remaining residue was extracted with dichloromethane, then the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* affording a red powder **13** (0.46 mmol, 91.0 % yield). Red crystals of **13** were obtained from a fluorobenzene solution layered with hexane on top and stored at –30 °C. M. P. = 185 °C. $^{1}H$ NMR (400 MHz, $C_6D_6$): δ = 7.45 (d, 1H, *J* = 7.2 Hz, $C_{ar}H$), 7.33 (d, 1H, *J* = 7.2 Hz, $C_{ar}H$), 7.14 (m, 4H, $C_{ar}H$), 7.01 (m, 3H, $C_{ar}H$), 6.81 (t, 1H, *J* = 7.6 Hz, $C_{ar}H$), 3.76 (m, 4H,

C*H*Me$_2$), 3.55 (m, 2H, C$H_2$), 3.19 (m, 2H, C$H_2$), 1.35 (d, 6H, $J$ = 6.8 Hz, $CH_3$), 1.26 (d, 6H, $J$ = 6.8 Hz, $CH_3$), 1.24 (d, 6H, $J$ = 7.2 Hz, $CH_3$), 1.26 (d, 6H, $J$ = 6.8 Hz, $CH_3$). $^{13}C\{H\}$ NMR (100.5 MHz, $C_6D_6$): δ = 223.6 (dd, $^1J_{CP}$ = 35.1 Hz, $^4J_{CP}$ = 15.8 Hz, *C*OPCOP), 218.8 (dd, $^1J_{CP}$ = 56.5 Hz, $^2J_{CP}$ = 18.9 Hz,, COP*C*OP), 150.0 (s, $C_{ar}$), 149.1 (d, $J_{CP}$ = 2.8 Hz, $C_{ar}$), 147.4 (d, $J_{CP}$ = 2.3 Hz, $C_{ar}$), 145.5 (d, $J_{CP}$ = 16.0 Hz, $C_{ar}$), 137.2 (t, $J_{CP}$ = 5.6 Hz, $C_{ar}$), 136.0 (s, $C_{ar}$), 135.9 (s, $C_{ar}$), 132.0 (d, $J_{CP}$ = 3.1 Hz, $C_{ar}$), 130.3 (d, $J_{CP}$ = 5.4 Hz, $C_{ar}$), 128.3 (s, $C_{ar}$), 124.4 (s, $C_{ar}$), 124.2 (s, $C_{ar}$), 120.1 (s, $C_{ar}$), 117.0 (d, $J_{CP}$ = 9.1 Hz, $C_{ar}$), 54.6 (d, $J_{CP}$ = 7.3 Hz, $CH_2$), 28.9, 28.9, 28.2, 25.3, 24.8, 24.6, 24.5, 24.2. $^{31}P\{H\}$ NMR (161.9 MHz, $C_6D_6$): δ = 126.9 (d, $J_{PP}$ = 100.9 Hz, PCO*P*N), 68.9 (d, $J_{PP}$ = 100.9 Hz, *P*COPN) . Elemental analysis (%): calcd for $C_{34}H_{42}N_2O_2P_2$; C 71.31, H 7.39; found: C 71.54, H 7.22. **IR** (ATR, [cm$^{-1}$]): 1651.0 (C=O).

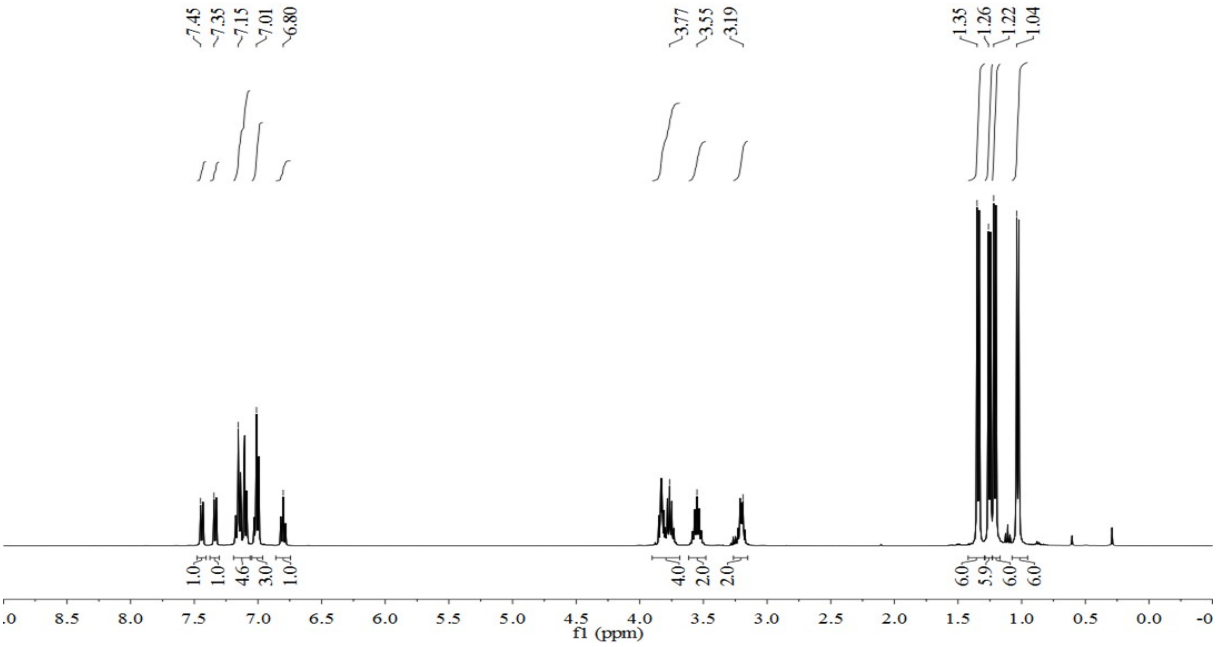



***Figure S37.*** $^1$H NMR spectrum of **13** in $C_6D_6$.

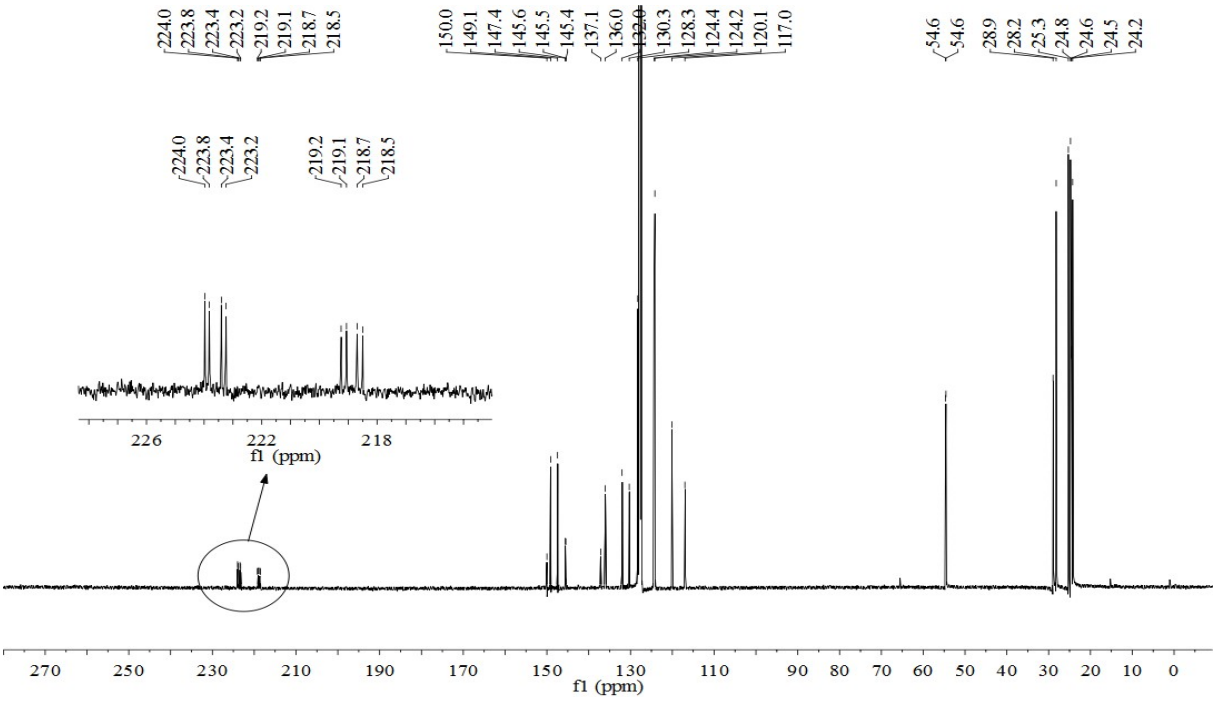



***Figure S38.*** $^{13}C\{^{1}H\}$ NMR spectrum of **13** in $C_6D_6$.

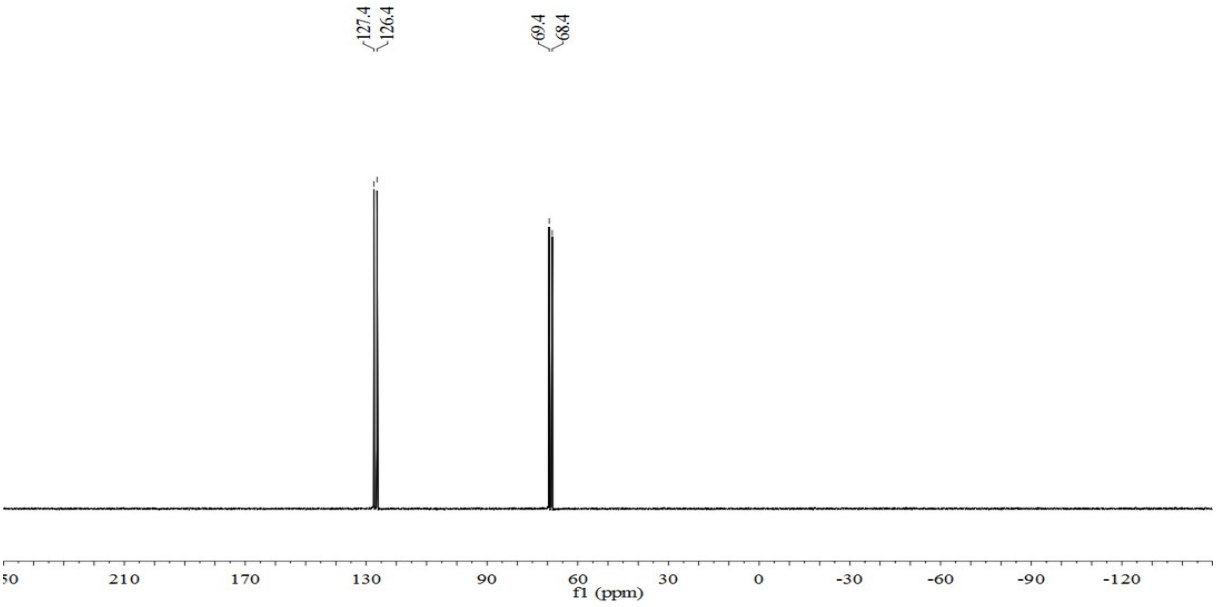



***Figure S39.*** $^{31}P\{^{1}H\}$ NMR spectrum of **13** in $C_6D_6$.

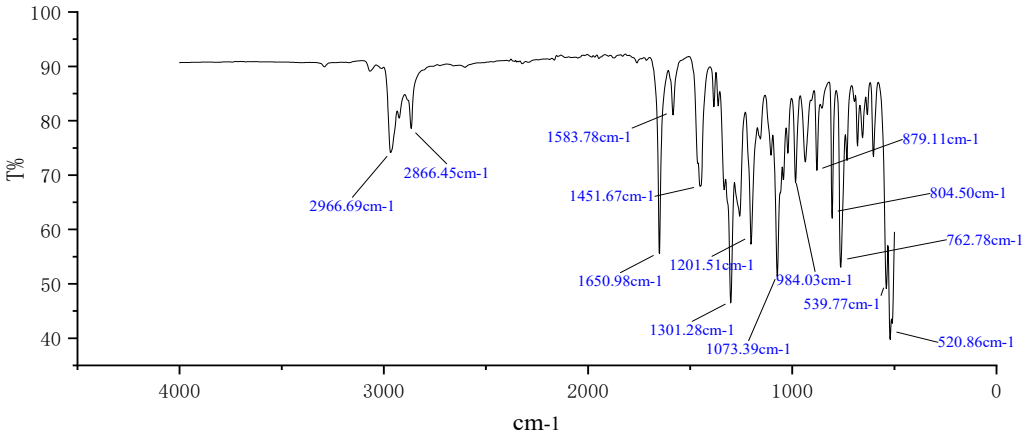



***Figure S40.*** IR spectrum of **13**

# S2: X-Ray Diffraction Studies

These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/cgi-bin/catreq.cgi, or by emailing data_request@ccdc.cam.ac.uk. The CCDC reference numbers are 1894664–1894672, 2162217.

**Table S1.** Crystal data and structure refinement for **1**[Na]. (CCDC 1894664)

| | |
|---|---|
| Empirical formula | $C_{48}H_{72}Na_3O_{18}P_3$ |
| Formula weight | 1098.987 |
| Temperature/K | 150.10(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 13.2833(3) |
| b/Å | 14.4071(3) |
| c/Å | 30.5777(8) |
| α/° | 90 |
| β/° | 100.568(2) |
| γ/° | 90 |
| Volume/Å$^3$ | 5752.5(2) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.269 |
| μ/mm$^{-1}$ | 1.731 |
| F(000) | 2340.8 |
| Crystal size/mm$^3$ | 0.06 × 0.03 × 0.03 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 6.76 to 142.28 |
| Index ranges | -16 ≤ h ≤ 16, -17 ≤ k ≤ 13, -32 ≤ l ≤ 37 |
| Reflections collected | 33361 |
| Independent reflections | 10920 [$R_{int}$ = 0.0419, $R_{sigma}$ = 0.0339] |
| Data/restraints/parameters | 10920/107/761 |
| Goodness-of-fit on $F^2$ | 1.021 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0479, $wR_2$ = 0.1302 |
| Final R indexes [all data] | $R_1$ = 0.0654, $wR_2$ = 0.1449 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.34/-0.37 |

**Table S2.** Crystal data and structure refinement for **1**-Me. (CCDC 1894665)

| | |
|---|---|
| Empirical formula | $C_9H_7O_2P$ |
| Formula weight | 178.12 |
| Temperature/K | 150.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 7.8469(2) |
| b/Å | 7.1421(2) |
| c/Å | 15.2070(4) |

| | |
|---|---|
| α/° | 90 |
| β/° | 100.147(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 838.92(4) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.410 |
| μ/mm$^{-1}$ | 2.528 |
| F(000) | 368.0 |
| Crystal size/mm$^3$ | 0.09 × 0.07 × 0.07 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 11.456 to 147.504 |
| Index ranges | -9 ≤ h ≤ 9, -8 ≤ k ≤ 7, -15 ≤ l ≤ 18 |
| Reflections collected | 4068 |
| Independent reflections | 1639 [$R_{int}$ = 0.0474, $R_{sigma}$ = 0.0477] |
| Data/restraints/parameters | 1639/0/110 |
| Goodness-of-fit on $F^2$ | 1.111 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0588, w$R_2$ = 0.1540 |
| Final R indexes [all data] | $R_1$ = 0.0608, w$R_2$ = 0.1568 |
| Largest diff. peak/hole / e Å$^{-3}$ | 1.08/-0.47 |

**Table S3.** Crystal data and structure refinement for **3**. (CCDC 1894666)

| | |
|---|---|
| Empirical formula | $C_{34}H_{42}N_2O_2PB$ |
| Formula weight | 552.47 |
| Temperature/K | 150.10(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 15.4261(2) |
| b/Å | 12.4164(2) |
| c/Å | 16.4259(2) |
| α/° | 90 |
| β/° | 96.0090(10) |
| γ/° | 90 |
| Volume/Å$^3$ | 3128.87(8) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.173 |
| μ/mm$^{-1}$ | 1.018 |
| F(000) | 1184.0 |
| Crystal size/mm$^3$ | 0.1 × 0.08 × 0.08 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 8.946 to 148.48 |
| Index ranges | -15 ≤ h ≤ 19, -15 ≤ k ≤ 13, -20 ≤ l ≤ 20 |
| Reflections collected | 18562 |
| Independent reflections | 6283 [$R_{int}$ = 0.0286, $R_{sigma}$ = 0.0250] |
| Data/restraints/parameters | 6283/1/369 |

| | |
|---|---|
| Goodness-of-fit on $F^2$ | 1.027 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0444, $wR_2$ = 0.1192 |
| Final R indexes [all data] | $R_1$ = 0.0480, $wR_2$ = 0.1242 |
| Largest diff. peak/hole / e $Å^{-3}$ | 0.39/-0.34 |

**Table S4.** Crystal data and structure refinement for **5**. (CCDC 1894667)

| | |
|---|---|
| Empirical formula | $C_{38}H_{48}AlN_2O_2P$ |
| Formula weight | 622.73 |
| Temperature/K | 150.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 13.08240(10) |
| b/Å | 20.5977(2) |
| c/Å | 13.70050(10) |
| α/° | 90 |
| β/° | 104.1500(10) |
| γ/° | 90 |
| Volume/$Å^3$ | 3579.82(5) |
| Z | 4 |
| $\rho_{calc}g/cm^3$ | 1.155 |
| $\mu/mm^{-1}$ | 1.173 |
| F(000) | 1336.0 |
| Crystal size/$mm^3$ | 0.11 × 0.1 × 0.09 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.92 to 148.364 |
| Index ranges | $-15 \le h \le 16$, $-21 \le k \le 25$, $-15 \le l \le 17$ |
| Reflections collected | 21246 |
| Independent reflections | 7076 [$R_{int}$ = 0.0295, $R_{sigma}$ = 0.0338] |
| Data/restraints/parameters | 7076/6/434 |
| Goodness-of-fit on $F^2$ | 1.066 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0392, $wR_2$ = 0.1057 |
| Final R indexes [all data] | $R_1$ = 0.0435, $wR_2$ = 0.1087 |
| Largest diff. peak/hole / e $Å^{-3}$ | 0.23/-0.45 |

**Table S5.** Crystal data and structure refinement for **6**. (CCDC 2162217)

| | |
|---|---|
| Empirical formula | $C_{27}H_{19}O_2P$ |
| Formula weight | 406.39 |
| Temperature/K | 150.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/n0$ |
| a/Å | 10.9231(2) |
| b/Å | 15.9165(3) |
| c/Å | 23.5573(4) |
| α/° | 90 |
| β/° | 92.171(2) |
| γ/° | 90 |
| Volume/$Å^3$ | 4092.67(13) |

| | |
|---|---|
| Z | 8 |
| $\rho_{calc}$g/cm$^3$ | 1.319 |
| μ/mm$^{-1}$ | 1.354 |
| F(000) | 1696.0 |
| Crystal size/mm$^3$ | 0.1 × 0.1 × 0.05 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 6.704 to 148.758 |
| Index ranges | -12 ≤ h ≤ 7, -19 ≤ k ≤ 18, -29 ≤ l ≤ 29 |
| Reflections collected | 20142 |
| Independent reflections | 7820 [$R_{int}$ = 0.0457, $R_{sigma}$ = 0.0529] |
| Data/restraints/parameters | 7820/0/541 |
| Goodness-of-fit on F$^2$ | 1.030 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0517, w$R_2$ = 0.1298 |
| Final R indexes [all data] | $R_1$ = 0.0733, w$R_2$ = 0.1440 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.40/-0.28 |

**Table S6.** Crystal data and structure refinement for **8**. (CCDC 1894668)

| | |
|---|---|
| Empirical formula | $C_{110}H_{81}FGe_4O_8P_4$ |
| Formula weight | 1964.208 |
| Temperature/K | 150 |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 17.5402(3) |
| b/Å | 8.8075(2) |
| c/Å | 30.5468(6) |
| α/° | 90 |
| β/° | 100.328(2) |
| γ/° | 90 |
| Volume/Å$^3$ | 4642.57(16) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.405 |
| μ/mm$^{-1}$ | 2.635 |
| F(000) | 2003.0 |
| Crystal size/mm$^3$ | 0.1 × 0.08 × 0.07 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.08 to 148.62 |
| Index ranges | -17 ≤ h ≤ 21, -10 ≤ k ≤ 10, -35 ≤ l ≤ 37 |
| Reflections collected | 26413 |
| Independent reflections | 9196 [$R_{int}$ = 0.0354, $R_{sigma}$ = 0.0307] |
| Data/restraints/parameters | 9196/0/590 |
| Goodness-of-fit on F$^2$ | 1.043 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0419, w$R_2$ = 0.1131 |
| Final R indexes [all data] | $R_1$ = 0.0463, w$R_2$ = 0.1179 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.53/-0.55 |

**Table S7.** Crystal data and structure refinement for **9**. (CCDC 1894672)

| | |
|---|---|
| Empirical formula | $C_{19}H_{16}NO_4P$ |
| Formula weight | 353.30 |
| Temperature/K | 100.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/m$ |
| a/Å | 10.3706(2) |
| b/Å | 14.3699(3) |
| c/Å | 11.4240(3) |
| α/° | 90 |
| β/° | 95.344(2) |
| γ/° | 90 |
| Volume/Å$^3$ | 1695.06(7) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.384 |
| μ/mm$^{-1}$ | 1.649 |
| F(000) | 736.0 |
| Crystal size/mm$^3$ | 0.06 × 0.06 × 0.03 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.772 to 130.066 |
| Index ranges | -11 ≤ h ≤ 12, -16 ≤ k ≤ 11, -12 ≤ l ≤ 13 |
| Reflections collected | 7327 |
| Independent reflections | 2907 [$R_{int}$ = 0.0130, $R_{sigma}$ = 0.0135] |
| Data/restraints/parameters | 2907/0/251 |
| Goodness-of-fit on $F^2$ | 1.035 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0290, $wR_2$ = 0.0765 |
| Final R indexes [all data] | $R_1$ = 0.0308, $wR_2$ = 0.0781 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.29/-0.29 |

**Table S8.** Crystal data and structure refinement for **10**. (CCDC 1894669)

| | |
|---|---|
| Empirical formula | $C_{16}H_8O_4P_2$ |
| Formula weight | 326.187 |
| Temperature/K | 100.00 |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 10.5737(4) |
| b/Å | 11.8608(3) |
| c/Å | 11.4453(4) |
| α/° | 90 |
| β/° | 100.127(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 1413.02(8) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.533 |

| | |
|---|---|
| μ/mm$^{-1}$ | 0.322 |
| F(000) | 665.2 |
| Crystal size/mm$^3$ | 0.12 × 0.11 × 0.08 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 5.94 to 65.38 |
| Index ranges | -15 ≤ h ≤ 15, -17 ≤ k ≤ 17, -17 ≤ l ≤ 17 |
| Reflections collected | 23212 |
| Independent reflections | 4867 [$R_{int}$ = 0.0485, $R_{sigma}$ = 0.0401] |
| Data/restraints/parameters | 4867/0/271 |
| Goodness-of-fit on $F^2$ | 1.110 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0452, $wR_2$ = 0.0712 |
| Final R indexes [all data] | $R_1$ = 0.0589, $wR_2$ = 0.0755 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.48/-0.42 |

**Table S9.** Crystal data and structure refinement for **11**. (CCDC 1894670)

| | |
|---|---|
| Empirical formula | $C_{20}H_{14}P_2O_2$ |
| Formula weight | 348.25 |
| Temperature/K | 150.00(10) |
| Crystal system | orthorhombic |
| Space group | $Pna2_1$ |
| a/Å | 12.7782(2) |
| b/Å | 10.31430(10) |
| c/Å | 13.0467(2) |
| α/° | 90.00 |
| β/° | 90.00 |
| γ/° | 90.00 |
| Volume/Å$^3$ | 1719.53(4) |
| Z | 4 |
| $ρ_{calc}$g/cm$^3$ | 1.345 |
| μ/mm$^{-1}$ | 2.367 |
| F(000) | 720.0 |
| Crystal size/mm$^3$ | 0.12 × 0.1 × 0.1 |
| Radiation | CuKα (λ = 1.54184) |
| 2Θ range for data collection/° | 10.94 to 148.62 |
| Index ranges | -12 ≤ h ≤ 15, -12 ≤ k ≤ 10, -15 ≤ l ≤ 15 |
| Reflections collected | 9100 |
| Independent reflections | 3350 [$R_{int}$ = 0.0323, $R_{sigma}$ = 0.0273] |
| Data/restraints/parameters | 3350/1/217 |
| Goodness-of-fit on $F^2$ | 1.041 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0356, $wR_2$ = 0.0912 |
| Final R indexes [all data] | $R_1$ = 0.0360, $wR_2$ = 0.0919 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.26/-0.27 |
| Flack parameter | -0.010(17) |

**Table S10.** Crystal data and structure refinement for **13**. (CCDC 1894671)

| | |
|---|---|
| Empirical formula | $C_{34}H_{42}N_2O_2P_2$ |
| Formula weight | 572.63 |
| Temperature/K | 100.01(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 11.1651(4) |
| b/Å | 16.2523(6) |
| c/Å | 17.4007(7) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90.01 |
| Volume/Å$^3$ | 3157.5(2) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.205 |
| μ/mm$^{-1}$ | 1.495 |
| F(000) | 1224.0 |
| Crystal size/mm$^3$ | 0.09 × 0.07 × 0.06 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 7.442 to 149.156 |
| Index ranges | -13 ≤ h ≤ 12, -12 ≤ k ≤ 20, -21 ≤ l ≤ 21 |
| Reflections collected | 20679 |
| Independent reflections | 6313 [$R_{int}$ = 0.0260, $R_{sigma}$ = 0.0216] |
| Data/restraints/parameters | 6313/0/369 |
| Goodness-of-fit on $F^2$ | 1.044 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0372, $wR_2$ = 0.1015 |
| Final R indexes [all data] | $R_1$ = 0.0394, $wR_2$ = 0.1033 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.45/-0.54 |

# S3: Theoretical Details

Geometry optimizations were performed using the Gaussian 09 optimizer[4]. All geometry optimizations were computed using the functional BP86[5] the BP86/def2-TZVP level of theory.[6] At each of the optimized structures vibrational analysis was performed to ensure that the geometry corresponds to an energy minimum. Natural Bond Orbital (NBO) for **1**, **PA** and **1**-Me were calculated by NBO 7.0 Program.[7] Main resonance structures and their relative weights were determined by Natural Resonance Theory (NRT), implemented within NBO 7.0 package.

**1: P5 anion**, E = -799.359788760

| | | | |
|---|---|---|---|
| P | 2.31849100 | -0.00000200 | 0.00002500 |
| O | 1.19870300 | 2.53812300 | 0.00001400 |
| O | 1.19870000 | -2.53812100 | 0.00000500 |
| C | 1.04035200 | -1.30387800 | -0.00000600 |
| C | 1.04035300 | 1.30387900 | -0.00001400 |
| C | -0.35082600 | -0.70029300 | -0.00006500 |
| C | -0.35082700 | 0.70029600 | -0.00006800 |
| C | -1.54965100 | 1.41083500 | -0.00001900 |
| H | -1.52162500 | 2.50371900 | 0.00004900 |
| C | -2.76359600 | 0.69992100 | 0.00003300 |
| H | -3.71436400 | 1.24159000 | 0.00002400 |
| C | -1.54964800 | -1.41083500 | -0.00001200 |
| H | -1.52162000 | -2.50371800 | 0.00006000 |
| C | -2.76359400 | -0.69992300 | 0.00003600 |
| H | -3.71436200 | -1.24159300 | 0.00003000 |

**PA: N5 anion**, E =-512.7470317

| | | | |
|---|---|---|---|
| O | -1.68878700 | -2.30581600 | 0.00021100 |
| O | -1.68878600 | 2.30581700 | 0.00022600 |
| C | -1.32577900 | 1.11843700 | -0.00008300 |
| C | -1.32578000 | -1.11843600 | -0.00008000 |
| C | 0.14293400 | 0.69726300 | -0.00006800 |
| C | 0.14293300 | -0.69726300 | -0.00006900 |
| C | 1.33047000 | -1.42042000 | -0.00002400 |
| H | 1.31555700 | -2.51399300 | -0.00001800 |
| C | 2.54025300 | -0.70141500 | 0.00001600 |
| H | 3.49414100 | -1.23770300 | 0.00005400 |
| C | 1.33047100 | 1.42041900 | -0.00002300 |
| H | 1.31555900 | 2.51399300 | -0.00001600 |
| C | 2.54025400 | 0.70141400 | 0.00001600 |
| H | 3.49414200 | 1.23770000 | 0.00005500 |
| N | -2.12190800 | 0.00000000 | -0.00024000 |

**1-Me: P5_O_Me**, E = -839.1866861

| | | | |
|---|---|---|---|
| P | 1.65567000 | 1.28892900 | -0.00016500 |
| O | -0.58101900 | 2.93854700 | 0.00018000 |
| O | 1.89882200 | -1.47169300 | 0.00009200 |
| C | 1.13820400 | -0.36817400 | -0.00002700 |
| C | -0.17785600 | 1.78836000 | 0.00000900 |
| C | -0.31682000 | -0.62128800 | -0.00009600 |
| C | -1.05886800 | 0.57202500 | -0.00004400 |
| C | -2.44789900 | 0.55616200 | 0.00003100 |
| H | -3.00071800 | 1.49765600 | 0.00009100 |
| C | -3.10728500 | -0.68494300 | 0.00003400 |
| H | -4.19828700 | -0.72175700 | 0.00008800 |
| C | -0.96731400 | -1.85589500 | -0.00007300 |
| H | -0.39681000 | -2.78549800 | -0.00007600 |
| C | -2.37232600 | -1.87419900 | -0.00001600 |
| H | -2.89617600 | -2.83223700 | -0.00000100 |
| C | 3.32523800 | -1.26899100 | 0.00014700 |
| H | 3.77316100 | -2.26857300 | 0.00012100 |
| H | 3.62548900 | -0.70836600 | -0.89888000 |
| H | 3.62541300 | -0.70833500 | 0.89916100 |

**1-Me: P5_P_Me**, E = -839.214077678

| | | | |
|---|---|---|---|
| P | 1.87432500 | -0.01011800 | -0.64983000 |
| O | 0.92815100 | 2.47369500 | 0.18934100 |
| O | 0.90644600 | -2.48627900 | 0.19515300 |
| C | 0.65631600 | -1.32294600 | -0.07397500 |
| C | 0.66630200 | 1.31183400 | -0.07600900 |
| C | -0.70604100 | -0.70357400 | -0.04301500 |
| C | -0.70089500 | 0.70457400 | -0.04339900 |
| C | -1.90042200 | 1.42133200 | 0.02260800 |
| H | -1.87883800 | 2.51256100 | 0.03149700 |
| C | -3.10214700 | 0.71236300 | 0.08473600 |
| H | -4.04906000 | 1.25318700 | 0.14055000 |
| C | -1.91087400 | -1.41132900 | 0.02337700 |
| H | -1.89732300 | -2.50268400 | 0.03300300 |
| C | -3.10731000 | -0.69342800 | 0.08509000 |
| H | -4.05816600 | -1.22727200 | 0.14116900 |
| C | 3.20861600 | 0.00730600 | 0.63679500 |
| H | 3.71140900 | 0.98278900 | 0.57881300 |
| H | 2.82057600 | -0.14593700 | 1.65125000 |
| H | 3.93848300 | -0.77698700 | 0.39796400 |

**3: P5_O_B**, E = -1947.172733

| | | | |
|---|---|---|---|
| P | 1.17687500 | 1.81467800 | -1.54938900 |
| O | -0.14102100 | 0.58286100 | 0.54629400 |
| O | 2.15757800 | 4.39451800 | -1.86985500 |
| N | -1.49182000 | -1.27596800 | -0.40831200 |
| N | 0.82508700 | -1.62793800 | -0.28101500 |
| C | 0.46555600 | 2.86394200 | 0.87635800 |
| C | 0.45480300 | 1.66011900 | 0.01936600 |
| C | -2.81602700 | -0.72881200 | -0.41374900 |
| C | 1.09517200 | 3.95523500 | 0.25326000 |
| C | -3.63881100 | -0.90531700 | 0.72801700 |
| C | 2.19450200 | -1.60913400 | 0.14121500 |
| C | 2.51544200 | -1.60976800 | 1.52413100 |
| C | -3.30637800 | -0.05536600 | -1.56160000 |
| C | -1.24778000 | -2.60369100 | -1.00523100 |

| | | | |
|---|---|---|---|
| H | -1.38626700 | -2.56550000 | -2.10094000 |
| H | -1.94854900 | -3.35492900 | -0.60818300 |
| C | -4.94068700 | -0.38505500 | 0.70456300 |
| H | -5.58232500 | -0.50770700 | 1.58048800 |
| C | 1.58289900 | 3.61591300 | -1.12691700 |
| C | -0.06832700 | 2.99871500 | 2.15816200 |
| H | -0.56633200 | 2.15810800 | 2.64242300 |
| C | 3.22465400 | -1.64070800 | -0.83705800 |
| C | 3.86758000 | -1.59870500 | 1.89884100 |
| H | 4.12684000 | -1.59004500 | 2.96012200 |
| C | 0.21597500 | -2.93133000 | -0.63502100 |
| H | 0.26742900 | -3.61365100 | 0.23380500 |
| H | 0.74745200 | -3.41408100 | -1.46768600 |
| C | -4.61856500 | 0.43958700 | -1.53592600 |
| H | -5.00893000 | 0.96271200 | -2.41180900 |
| C | 1.45819300 | -1.67425700 | 2.62176600 |
| H | 0.46816500 | -1.61004500 | 2.14472100 |
| C | -3.15597900 | -1.64270700 | 1.97136700 |
| H | -2.12583700 | -1.97570900 | 1.77306300 |
| C | -2.46699600 | 0.13123500 | -2.82044100 |
| H | -1.44207700 | -0.19951000 | -2.58968000 |
| C | 1.20918800 | 5.18239400 | 0.89243200 |
| H | 1.70307100 | 6.01373300 | 0.38548500 |
| C | -5.43192900 | 0.28160000 | -0.41582100 |
| H | -6.44950700 | 0.67823800 | -0.41644100 |
| C | 4.88422000 | -1.61480700 | 0.94805000 |
| H | 5.93029800 | -1.60861200 | 1.26159700 |
| C | 0.67653000 | 5.32064300 | 2.18659700 |
| H | 0.75381600 | 6.27672300 | 2.70780700 |
| C | 4.55805400 | -1.64500400 | -0.40630800 |
| H | 5.35836100 | -1.66376600 | -1.14919600 |
| C | 0.04449400 | 4.24010500 | 2.80785900 |
| H | -0.36926200 | 4.36043100 | 3.81115000 |
| C | 1.57034700 | -0.50006000 | 3.61083100 |
| H | 2.52038200 | -0.53197900 | 4.16616300 |
| H | 0.75475300 | -0.54038500 | 4.34933900 |
| H | 1.51785100 | 0.46695600 | 3.09156200 |
| C | 2.92853200 | -1.69715500 | -2.33198600 |
| H | 1.85434500 | -1.48983900 | -2.45837600 |
| C | -2.38336000 | 1.60673700 | -3.25166700 |
| H | -3.36858900 | 1.99820800 | -3.54888700 |
| H | -1.70884800 | 1.71345700 | -4.11455500 |
| H | -1.99488300 | 2.23930300 | -2.44117100 |
| C | -2.99805200 | -0.73929000 | -3.97799900 |
| H | -3.04495300 | -1.80298300 | -3.70045500 |
| H | -2.34928800 | -0.64329400 | -4.86234500 |
| H | -4.01333000 | -0.42839000 | -4.27051000 |
| B | -0.23871900 | -0.69829600 | -0.05473100 |
| C | -4.00639400 | -2.89534400 | 2.25820900 |
| H | -5.04833600 | -2.62835100 | 2.49385400 |
| H | -3.60118600 | -3.44802000 | 3.12007100 |
| H | -4.02554800 | -3.57568200 | 1.39385200 |
| C | 1.51885800 | -3.02231000 | 3.36917800 |
| H | 1.40763800 | -3.87164100 | 2.67887100 |
| H | 0.71757000 | -3.08399100 | 4.12202300 |
| H | 2.48043800 | -3.14285100 | 3.89180500 |
| C | -3.11523100 | -0.71543900 | 3.20068600 |
| H | -2.48142200 | 0.16343300 | 3.01400300 |
| H | -2.71513800 | -1.25001100 | 4.07623800 |
| H | -4.12165900 | -0.35313600 | 3.46206500 |
| C | 3.70117200 | -0.63178500 | -3.13083900 |
| H | 3.51504000 | 0.37609600 | -2.73530800 |
| H | 3.38660600 | -0.64741200 | -4.18569700 |
| H | 4.78650000 | -0.81557000 | -3.10913300 |
| C | 3.22770400 | -3.09967300 | -2.90366300 |
| H | 4.30329000 | -3.32665600 | -2.83455300 |
| H | 2.94070700 | -3.15452000 | -3.96540100 |
| H | 2.69072700 | -3.89257500 | -2.36188100 |

**3: P5_P_B**, E = -1947.155934

| | | | |
|---|---|---|---|
| N | -0.30043500 | -1.30826300 | -0.93498300 |
| N | 1.87949000 | -0.55984300 | -0.55821400 |
| C | -1.71456800 | -1.53293000 | -1.00615500 |
| C | -2.26743300 | -2.65373900 | -0.33336200 |
| C | 3.07846300 | -0.01342100 | 0.00680000 |
| C | 3.55905900 | -0.49109900 | 1.25410700 |
| C | -2.53425100 | -0.68432700 | -1.79515000 |
| C | 0.55735600 | -2.01205000 | -1.92084500 |
| H | 0.35171900 | -1.62739800 | -2.93553600 |
| H | 0.34694700 | -3.09228700 | -1.92739400 |
| C | -3.64760600 | -2.87791400 | -0.42960600 |
| H | -4.08760200 | -3.73034600 | 0.09288300 |
| C | 3.79867300 | 0.96951100 | -0.71945700 |
| C | 4.74352200 | 0.05832900 | 1.76660000 |
| H | 5.12148400 | -0.29260400 | 2.72971500 |
| C | 2.00372300 | -1.70644300 | -1.48436100 |
| H | 2.46112100 | -2.56333000 | -0.95596300 |
| H | 2.65073900 | -1.46377500 | -2.34138200 |
| C | -3.91017600 | -0.95286700 | -1.85384800 |
| H | -4.55566900 | -0.30475700 | -2.45056400 |
| C | 2.86223300 | -1.59853100 | 2.03779600 |
| H | 1.92096100 | -1.83570400 | 1.51819300 |
| C | -1.40860100 | -3.63713900 | 0.45475400 |
| H | -0.39068100 | -3.22001100 | 0.49660100 |
| C | -1.96491300 | 0.46056600 | -2.62679100 |
| H | -0.93937600 | 0.65183300 | -2.27548400 |
| C | -4.46777800 | -2.03412500 | -1.17526300 |
| H | -5.54192100 | -2.22334400 | -1.23360100 |
| C | 5.45083300 | 1.03555200 | 1.07001900 |
| H | 6.37129800 | 1.44909100 | 1.48791200 |
| C | 4.98072800 | 1.47926000 | -0.16427600 |
| H | 5.54124000 | 2.24222000 | -0.70939500 |
| C | 2.49982800 | -1.16309800 | 3.46971200 |
| H | 3.40104400 | -0.95625200 | 4.06755600 |
| H | 1.93689300 | -1.95875000 | 3.98117700 |
| H | 1.88080200 | -0.25441700 | 3.46388500 |
| C | 3.34127300 | 1.46977900 | -2.08500200 |
| H | 2.36166200 | 1.01144400 | -2.28925800 |
| C | -2.76000700 | 1.76925000 | -2.47454500 |
| H | -3.76316600 | 1.68813000 | -2.92124400 |
| H | -2.23719200 | 2.59203300 | -2.98431500 |
| H | -2.88459000 | 2.04916400 | -1.41956100 |
| C | -1.88786800 | 0.06638100 | -4.11774600 |
| H | -1.30416500 | -0.85335400 | -4.26963200 |
| H | -1.42040300 | 0.87074300 | -4.70686100 |
| H | -2.89569500 | -0.11053900 | -4.52555300 |
| B | 0.50743100 | -0.39616800 | -0.19125900 |
| C | -1.33568600 | -5.00192000 | -0.26160100 |
| H | -2.32789300 | -5.47830200 | -0.30204300 |
| H | -0.65821500 | -5.68425000 | 0.27520900 |
| H | -0.97481900 | -4.90527400 | -1.29682500 |
| C | 3.71649300 | -2.88278000 | 2.06079500 |
| H | 3.96156100 | -3.22481900 | 1.04411300 |
| H | 3.17989800 | -3.69433200 | 2.57640200 |
| H | 4.66618600 | -2.71685400 | 2.59297300 |
| C | -1.89305800 | -3.81675600 | 1.90514500 |
| H | -1.93814700 | -2.85296600 | 2.42866000 |
| H | -1.20843400 | -4.48393900 | 2.45215200 |
| H | -2.89403800 | -4.27476900 | 1.94064000 |
| C | 3.14559500 | 2.99672400 | -2.11022200 |
| H | 2.40369900 | 3.31319200 | -1.36487300 |
| H | 2.78804900 | 3.31645100 | -3.10154800 |
| H | 4.09025300 | 3.52716200 | -1.91258000 |
| C | 4.31768600 | 1.02701700 | -3.19404100 |
| H | 5.30877400 | 1.48720300 | -3.05622600 |

| | | | |
|---|---|---|---|
| H | 3.94198600 | 1.33223900 | -4.18312700 |
| H | 4.45955500 | -0.06443800 | -3.20313100 |
| P | 0.04853200 | 0.88909700 | 1.20093100 |
| C | -0.53304000 | 2.48688000 | 0.41282600 |
| C | -1.65567000 | 0.59129800 | 1.91458300 |
| O | 0.03165600 | 3.15153100 | -0.44089800 |
| C | -1.80939200 | 2.88928900 | 1.08791700 |
| O | -2.07211700 | -0.42455900 | 2.44776600 |
| C | -2.40635100 | 1.88733800 | 1.87033200 |
| C | -2.40578300 | 4.14775100 | 0.96496600 |
| C | -3.61077000 | 2.12750200 | 2.53751300 |
| H | -1.92764900 | 4.91413300 | 0.35240700 |
| C | -3.61149200 | 4.38694400 | 1.63060700 |
| H | -4.06160100 | 1.33493200 | 3.13730500 |
| C | -4.21067300 | 3.38355000 | 2.40933400 |
| H | -4.09565300 | 5.36168600 | 1.54236100 |
| H | -5.15585800 | 3.58780700 | 2.91650100 |

**5: P5_O_Al**, E = -2320.841352

| | | | |
|---|---|---|---|
| Al | -0.48774700 | 0.00013400 | -0.61683400 |
| P | 2.55946600 | 0.00004000 | 1.70912800 |
| O | 1.31468800 | 0.00084200 | -0.75501200 |
| N | -1.02169300 | 1.45699500 | 0.51619100 |
| N | -1.02106100 | -1.45718100 | 0.51601800 |
| C | -1.29579200 | 2.77084600 | -0.04277900 |
| C | -1.09918400 | -1.27132500 | 1.85029700 |
| C | -2.62442100 | 3.07833400 | -0.43965700 |
| C | -1.29486800 | -2.77111600 | -0.04290300 |
| C | -0.25392600 | 3.71623400 | -0.21464300 |
| C | -1.09978300 | 1.27106200 | 1.85045300 |
| O | 5.23601200 | -0.00032800 | 2.44700500 |
| C | -0.25268000 | -3.71607100 | -0.21520200 |
| C | -2.62354200 | -3.07916600 | -0.43912800 |
| C | 2.41112500 | 0.00047900 | -0.03770500 |
| C | -2.88415200 | 4.34446000 | -0.98287100 |
| H | -3.90319000 | 4.59642500 | -1.28302400 |
| C | -1.19131300 | -0.00016800 | -2.44365600 |
| H | -0.84400100 | 0.88454700 | -3.00163300 |
| H | -2.29083000 | -0.00002700 | -2.49144700 |
| H | -0.84425600 | -0.88528400 | -3.00114800 |
| C | -0.56992600 | -4.96430700 | -0.77332300 |
| H | 0.22608700 | -5.69957900 | -0.90975600 |
| C | -0.57144900 | 4.96434600 | -0.77290700 |
| H | 0.22432300 | 5.69994400 | -0.90897000 |
| C | -1.06142700 | -0.00015100 | 2.45309400 |
| H | -1.07636900 | -0.00024200 | 3.54154200 |
| C | 1.19528800 | 3.44331900 | 0.16875300 |
| H | 1.24770000 | 2.45357800 | 0.64687200 |
| C | -2.88299900 | -4.34543300 | -0.98217200 |
| H | -3.90209000 | -4.59783700 | -1.28178400 |
| C | -3.78287700 | -2.10159300 | -0.26847400 |
| H | -3.35312400 | -1.10895700 | -0.06374400 |
| C | -3.78340800 | 2.10029700 | -0.26941300 |
| H | -3.35331900 | 1.10769700 | -0.06520800 |
| C | -1.87136300 | 5.28583800 | -1.15029000 |
| H | -2.09547300 | 6.26553100 | -1.57731000 |
| C | -1.22139900 | -2.46022900 | 2.77177600 |
| H | -1.88970800 | -3.22984200 | 2.36487800 |
| H | -1.57810400 | -2.15323400 | 3.76182300 |
| H | -0.23178700 | -2.92850700 | 2.89678400 |
| C | -1.22268900 | 2.45986400 | 2.77194000 |
| H | -0.23348300 | 2.92904900 | 2.89665000 |
| H | -1.57886200 | 2.15257500 | 3.76208700 |
| H | -1.89181400 | 3.22887100 | 2.36519300 |
| C | 3.70186600 | 0.00062200 | -0.77876100 |
| C | -1.86989100 | -5.28636900 | -1.15007700 |
| H | -2.09376400 | -6.26617300 | -1.57696800 |
| C | 1.19655600 | -3.44256100 | 0.16769100 |
| H | 1.24871400 | -2.45278400 | 0.64574700 |
| C | 4.82013400 | 0.00030900 | 0.07051100 |
| C | 1.73521600 | 4.47147700 | 1.18218900 |
| H | 1.79979700 | 5.47801500 | 0.74059800 |
| H | 2.74607400 | 4.18456200 | 1.50844300 |
| H | 1.09782800 | 4.54229100 | 2.07580100 |
| C | 2.09775400 | 3.40716700 | -1.08017000 |
| H | 1.74968300 | 2.66045200 | -1.80745000 |
| H | 3.13100300 | 3.15367200 | -0.80013100 |
| H | 2.11548200 | 4.38697500 | -1.58277400 |
| C | 3.86993600 | 0.00104300 | -2.16352700 |
| H | 3.00074300 | 0.00129500 | -2.82294200 |
| C | 4.43263900 | -0.00009200 | 1.52463400 |
| C | -4.64162000 | 1.98346800 | -1.54184400 |
| H | -5.17232600 | 2.92167900 | -1.76394900 |
| H | -5.40581000 | 1.20232800 | -1.41377500 |
| H | -4.03078500 | 1.72572400 | -2.41864300 |
| C | -4.66624000 | 2.47905800 | 0.93752800 |
| H | -4.09346800 | 2.49296900 | 1.87558000 |
| H | -5.48972800 | 1.75783800 | 1.05565100 |
| H | -5.10907500 | 3.47790000 | 0.79916200 |
| C | 2.09857000 | -3.40611700 | -1.08154300 |
| H | 2.11630300 | -4.38584700 | -1.58428800 |
| H | 3.13186300 | -3.15244900 | -0.80183800 |
| H | 1.75008200 | -2.65938000 | -1.80860500 |
| C | -4.66570700 | -2.48123100 | 0.93818100 |
| H | -5.10843500 | -3.48002700 | 0.79918600 |
| H | -5.48927500 | -1.76018000 | 1.05673500 |
| H | -4.09295000 | -2.49567300 | 1.87623200 |
| C | 6.11221600 | 0.00040000 | -0.44021600 |
| H | 6.96451200 | 0.00015700 | 0.24242200 |
| C | 1.73716900 | -4.47045200 | 1.18102200 |
| H | 1.10012100 | -4.54131800 | 2.07487400 |
| H | 2.74806800 | -4.18323000 | 1.50688000 |
| H | 1.80185500 | -5.47703300 | 0.73953800 |
| C | 6.28581900 | 0.00080800 | -1.83554500 |
| H | 7.29218500 | 0.00089600 | -2.25910600 |
| C | 5.17497000 | 0.00112900 | -2.68477400 |
| H | 5.32272300 | 0.00144700 | -3.76685300 |
| C | -4.64093400 | -1.98443800 | -1.54097900 |
| H | -4.03010200 | -1.72557200 | -2.41745100 |
| H | -5.40575000 | -1.20397400 | -1.41249000 |
| H | -5.17085800 | -2.92288700 | -1.76392800 |

**5: P5_P_Al**, E = -2320.814559

| | | | |
|---|---|---|---|
| Al | -0.26881800 | 0.15057700 | -0.51463300 |
| N | -1.71470200 | 0.94922200 | 0.48788600 |
| N | -0.13825800 | -1.50410600 | 0.45232300 |
| C | -2.67181700 | 1.88253800 | -0.08031800 |
| C | -0.21759000 | -1.35470800 | 1.79606400 |
| C | -3.86047100 | 1.37892200 | -0.66912400 |
| C | 0.10163300 | -2.81463000 | -0.11953500 |
| C | -2.40638900 | 3.27811400 | -0.07909100 |
| C | -1.69871900 | 0.71677100 | 1.81331900 |
| C | 1.32569700 | -3.11136400 | -0.77082400 |
| C | -0.92645300 | -3.79659100 | -0.05092200 |
| C | -4.77385200 | 2.28724500 | -1.22405600 |
| H | -5.69602300 | 1.90805100 | -1.66926900 |
| C | -0.49780900 | 0.10487700 | -2.46189800 |
| H | -1.34013300 | 0.74448000 | -2.77065600 |
| H | -0.70331000 | -0.91452800 | -2.82586800 |
| H | 0.39522600 | 0.47797100 | -2.98507900 |
| C | 1.49970600 | -4.38598500 | -1.33101700 |
| H | 2.44335800 | -4.61826300 | -1.82914900 |
| C | -3.35389100 | 4.13747600 | -0.65570800 |

| | | | |
|---|---|---|---|
| H | -3.15601400 | 5.21137400 | -0.66201900 |
| C | -0.86394700 | -0.25888200 | 2.40281700 |
| H | -0.82767800 | -0.24689700 | 3.49139300 |
| C | -1.13287700 | 3.89786800 | 0.48600800 |
| H | -0.55536300 | 3.10878500 | 0.99096200 |
| C | -0.68841700 | -5.05887800 | -0.61293900 |
| H | -1.46967100 | -5.81994700 | -0.55531500 |
| C | -2.29063100 | -3.55075900 | 0.59060300 |
| H | -2.35179500 | -2.48945800 | 0.87308800 |
| C | -4.20924800 | -0.10510700 | -0.70312400 |
| H | -3.32802900 | -0.66743200 | -0.35840800 |
| C | -4.53149700 | 3.65743000 | -1.21998700 |
| H | -5.25446600 | 4.34737600 | -1.65996700 |
| C | 0.43200700 | -2.35584400 | 2.71938300 |
| H | 0.59505700 | -3.32696000 | 2.23975700 |
| H | -0.14948700 | -2.49352700 | 3.63988200 |
| H | 1.41446900 | -1.93946300 | 2.99928400 |
| C | -2.59680800 | 1.50685400 | 2.73280800 |
| H | -2.26028700 | 2.55251900 | 2.79998900 |
| H | -2.59937400 | 1.07656000 | 3.74074300 |
| H | -3.62672200 | 1.53344900 | 2.34937800 |
| C | 0.51106000 | -5.36093000 | -1.25134600 |
| H | 0.67209000 | -6.34947900 | -1.68617900 |
| C | 2.48928900 | -2.13297600 | -0.85288700 |
| H | 2.16411300 | -1.17772500 | -0.41244400 |
| C | -1.41975700 | 5.00334600 | 1.52106300 |
| H | -1.89717200 | 5.88031600 | 1.05747600 |
| H | -0.47825600 | 5.34413900 | 1.97765100 |
| H | -2.08268600 | 4.65625800 | 2.32802500 |
| C | -0.24621400 | 4.45184000 | -0.64660500 |
| H | 0.02482100 | 3.67578600 | -1.37719000 |
| H | 0.68837700 | 4.86156200 | -0.23498600 |
| H | -0.76248900 | 5.25856900 | -1.19058900 |
| C | -4.54128300 | -0.58204300 | -2.12951000 |
| H | -5.43482800 | -0.07807700 | -2.52780100 |
| H | -4.74668100 | -1.66256400 | -2.13441600 |
| H | -3.70911800 | -0.38733800 | -2.82101500 |
| C | -5.37144800 | -0.42019900 | 0.26032300 |
| H | -5.12733000 | -0.14245800 | 1.29630700 |
| H | -5.60947300 | -1.49469800 | 0.24396600 |
| H | -6.28108700 | 0.12954500 | -0.02737700 |
| C | 2.91291300 | -1.85364500 | -2.30699200 |
| H | 3.30901400 | -2.75949500 | -2.79169800 |
| H | 3.70516700 | -1.09071100 | -2.33288000 |
| H | 2.07016500 | -1.48923100 | -2.91108600 |
| C | -2.48934100 | -4.38905300 | 1.86962200 |
| H | -2.46258400 | -5.46604900 | 1.64163800 |
| H | -3.46661800 | -4.16777100 | 2.32592700 |
| H | -1.71126300 | -4.18735400 | 2.61824300 |
| C | 3.68795400 | -2.63182100 | -0.02106300 |
| H | 3.41413500 | -2.77627000 | 1.03357000 |
| H | 4.51137800 | -1.90332900 | -0.06025500 |
| H | 4.06577400 | -3.59055700 | -0.40973100 |
| C | -3.43112200 | -3.83534700 | -0.40529400 |
| H | -3.30208700 | -3.26668800 | -1.33659900 |
| H | -4.40227500 | -3.56470300 | 0.03634900 |
| H | -3.47730500 | -4.90262800 | -0.66978800 |
| P | 1.60056900 | 1.53150400 | 0.27787000 |
| C | 2.80860600 | 1.95919700 | -1.05888900 |
| C | 2.92537300 | 0.74121500 | 1.29973100 |
| O | 2.56280000 | 2.40256100 | -2.17539800 |
| C | 4.20159800 | 1.74000500 | -0.53586800 |
| O | 2.79290500 | 0.06807400 | 2.31850300 |
| C | 4.26170300 | 1.10520000 | 0.71501300 |
| C | 5.37018000 | 2.11658900 | -1.19995100 |
| C | 5.49193400 | 0.84225400 | 1.32105100 |
| H | 5.30237400 | 2.60669000 | -2.17310000 |
| C | 6.60480800 | 1.85133400 | -0.59453000 |
| H | 5.51926700 | 0.34717500 | 2.29359100 |
| C | 6.66507300 | 1.22050300 | 0.65660900 |
| H | 7.52987400 | 2.13635700 | -1.10019200 |
| H | 7.63641400 | 1.02079900 | 1.11409700 |

**5$^{M}$: P5_O_Al$^{M}$**, E = -1466.014969Al -1.46860800 1.39462000 0.10646900

| | | | |
|---|---|---|---|
| P | 0.69156400 | -1.52151600 | -0.08570900 |
| O | 0.33048400 | 1.21349600 | 0.06117800 |
| N | -2.18392700 | 0.28242200 | 1.46692000 |
| N | -2.23734400 | 0.52399500 | -1.39422200 |
| C | -2.97848200 | -0.59214400 | -1.30425800 |
| C | -2.92820800 | -0.80691200 | 1.21837600 |
| O | 2.97313900 | -3.10080100 | -0.17715300 |
| C | 1.13161800 | 0.17197400 | 0.00091900 |
| C | -1.84031800 | 3.31761300 | 0.27355400 |
| H | -1.38107600 | 3.75235200 | 1.17672400 |
| H | -2.92040600 | 3.52963500 | 0.32603000 |
| H | -1.43909200 | 3.89269200 | -0.57742000 |
| C | -3.30701700 | -1.20039400 | -0.07872700 |
| H | -3.91138200 | -2.10318300 | -0.14346900 |
| C | -3.48805700 | -1.24338700 | -2.56579000 |
| H | -4.10738100 | -0.54733300 | -3.15357700 |
| H | -4.08831900 | -2.12996200 | -2.33352600 |
| H | -2.65121700 | -1.55197000 | -3.21237500 |
| C | -3.38852000 | -1.66532600 | 2.36998000 |
| H | -2.52835800 | -2.05490700 | 2.93676900 |
| H | -3.97967100 | -2.51511700 | 2.01159800 |
| H | -4.00404300 | -1.08732800 | 3.07740300 |
| C | 2.59237800 | 0.44643900 | 0.00609800 |
| C | 3.36649700 | -0.72333100 | -0.05875900 |
| C | 3.20757700 | 1.69673000 | 0.06812600 |
| H | 2.60361200 | 2.60403200 | 0.11980100 |
| C | 2.51852000 | -1.96657500 | -0.11763700 |
| C | 4.75422700 | -0.66804600 | -0.06333900 |
| H | 5.33325300 | -1.59251800 | -0.11399900 |
| C | 5.37913300 | 0.59046700 | -0.00177100 |
| H | 6.46900400 | 0.65773000 | -0.00429900 |
| C | 4.61187100 | 1.75740500 | 0.06330900 |
| H | 5.10962100 | 2.72841400 | 0.11142300 |
| C | -1.92967000 | 1.07811900 | -2.71799800 |
| H | -1.33306800 | 0.38082100 | -3.32841700 |
| H | -2.84121100 | 1.33843200 | -3.28022800 |
| H | -1.34239900 | 1.99844100 | -2.59471100 |
| C | -1.80952600 | 0.59948200 | 2.84992000 |
| H | -2.68854300 | 0.69824100 | 3.50699800 |
| H | -1.13882000 | -0.16393200 | 3.27763300 |
| H | -1.27428700 | 1.55898500 | 2.86606200 |

**5$^{M}$: P5_P_Al$^{M}$**, E =-1465.99595567

| | | | |
|---|---|---|---|
| Al | 1.58008300 | -0.89192000 | -0.81344500 |
| P | -0.52376600 | -0.24580000 | -1.86311500 |
| O | -0.50126700 | 2.37088300 | -0.92814400 |
| N | 1.39685500 | -1.35096600 | 1.02484100 |
| N | 2.48364900 | 0.76537000 | -0.58923800 |
| C | 2.68836300 | 1.34034000 | 0.60396800 |
| C | 1.77172900 | -0.54315600 | 2.02982400 |
| O | -1.96662200 | -2.47627400 | -1.03185400 |
| C | -1.06183700 | 1.27839800 | -0.94174800 |
| C | 2.46670000 | -2.27667800 | -1.89916000 |
| H | 1.81879400 | -3.15561900 | -2.04870900 |
| H | 3.40134300 | -2.62879400 | -1.43234200 |
| H | 2.71960300 | -1.90596200 | -2.90587400 |
| C | 2.36639600 | 0.71597700 | 1.82615800 |
| H | 2.60190600 | 1.28238900 | 2.72540700 |
| C | 3.28626400 | 2.72366900 | 0.66180700 |
| H | 4.27470200 | 2.75339400 | 0.17692900 |
| H | 3.39835100 | 3.05947500 | 1.69869800 |

| | | | |
|---|---|---|---|
| H | 2.64356000 | 3.44134800 | 0.12799600 |
| C | 1.55188000 | -0.98870800 | 3.45520900 |
| H | 0.48232000 | -1.15927500 | 3.65637500 |
| H | 1.92132400 | -0.23662100 | 4.16123900 |
| H | 2.06813700 | -1.94036600 | 3.65790800 |
| C | -2.35818100 | 1.00471700 | -0.23334400 |
| C | -2.76746700 | -0.33714900 | -0.26918200 |
| C | -3.12468700 | 1.96551000 | 0.43009500 |
| H | -2.78879700 | 3.00414100 | 0.44812200 |
| C | -1.83330100 | -1.25741800 | -1.00516400 |
| C | -3.94901000 | -0.73832900 | 0.35857700 |
| H | -4.25013800 | -1.78709800 | 0.32110000 |
| C | -4.71918900 | 0.22385100 | 1.02196000 |
| H | -5.64722000 | -0.07025800 | 1.51699700 |
| C | -4.30989700 | 1.56567300 | 1.05774700 |
| H | -4.92319700 | 2.30267300 | 1.58072800 |
| C | 2.80882000 | 1.50913400 | -1.81283800 |
| H | 2.15569600 | 2.38906600 | -1.92867800 |
| H | 3.86107400 | 1.83500100 | -1.83207600 |
| H | 2.64770300 | 0.85680400 | -2.68245800 |
| C | 0.78988500 | -2.65260700 | 1.33332700 |
| H | 1.49458600 | -3.31958900 | 1.85770900 |
| H | -0.11586800 | -2.55100500 | 1.95165200 |
| H | 0.49230400 | -3.14477700 | 0.39813100 |

**6: P5_O_CPh$_3$**, E =-1532.5444816

| | | | |
|---|---|---|---|
| P | 1.74062200 | -1.69023100 | 0.36129800 |
| O | 0.25686000 | 0.67547600 | 0.00959700 |
| O | 4.48064200 | -2.08972900 | 0.54216700 |
| C | -1.05385000 | -1.07843600 | -1.09888000 |
| C | -2.00227700 | 1.20537200 | -0.46183200 |
| C | -1.52435100 | -0.39975300 | 1.36565700 |
| C | -1.37469100 | -2.41334600 | -0.82177600 |
| H | -1.65244000 | -2.70789100 | 0.18997300 |
| C | -0.65938100 | -0.73799300 | -2.40575700 |
| H | -0.39759200 | 0.29668300 | -2.63542000 |
| C | 3.58952800 | -1.27259400 | 0.37453700 |
| C | 1.41194600 | -0.00314400 | 0.11383900 |
| C | -0.92792600 | -3.03473600 | -3.12214800 |
| H | -0.87765900 | -3.79380000 | -3.90522700 |
| C | -0.71676700 | -0.21596900 | 2.49552100 |
| H | 0.28349600 | 0.20140800 | 2.39374800 |
| C | 3.80639200 | 0.19552400 | 0.15540200 |
| C | -1.31888400 | -3.38318200 | -1.82862300 |
| H | -1.56870600 | -4.41892600 | -1.59092800 |
| C | -0.59166600 | -1.70637700 | -3.40656800 |
| H | -0.27566300 | -1.42347700 | -4.41258400 |
| C | 2.59398200 | 0.88962000 | 0.01070400 |
| C | -1.81781100 | 2.46947200 | 0.12234500 |
| H | -1.00248500 | 2.62209700 | 0.83027700 |
| C | -2.81971800 | -0.91665300 | 1.54613800 |
| H | -3.48264700 | -1.03055600 | 0.68652500 |
| C | -3.07185800 | 1.02321200 | -1.34875200 |
| H | -3.23387500 | 0.04979200 | -1.81349800 |
| C | -1.18143900 | -0.56515900 | 3.76866900 |
| H | -0.53163600 | -0.41762600 | 4.63348800 |
| C | -3.73120300 | 3.34139800 | -1.08337400 |
| H | -4.39875300 | 4.17021300 | -1.32684300 |
| C | -2.46003600 | -1.09856400 | 3.93458300 |
| H | -2.81970000 | -1.37138900 | 4.92846700 |
| C | -3.93178200 | 2.08386700 | -1.65504400 |
| H | -4.75815000 | 1.92209900 | -2.35014700 |
| C | -2.66875300 | 3.52965400 | -0.19280800 |
| H | -2.50472700 | 4.50720000 | 0.26536500 |
| C | -3.28056600 | -1.26967700 | 2.81505100 |
| H | -4.28962900 | -1.67082800 | 2.92896800 |
| C | 2.59760800 | 2.26778300 | -0.21115100 |
| H | 1.66110200 | 2.81319400 | -0.33283600 |
| C | 5.02790300 | 0.85251000 | 0.08419100 |
| H | 5.95410700 | 0.28562400 | 0.19848500 |
| C | 5.03593500 | 2.24086300 | -0.13561600 |
| H | 5.98426000 | 2.77856600 | -0.19316300 |
| C | 3.83229900 | 2.93590700 | -0.28207500 |
| H | 3.84890900 | 4.01396900 | -0.45534000 |
| C | -1.08722900 | 0.03392500 | -0.04438200 |

**6: P5_P_CPh$_3$**, E =-1532.5657335

| | | | |
|---|---|---|---|
| P | -0.47230500 | 0.04976600 | -1.22486900 |
| O | -1.49506700 | 2.53533700 | -0.41021600 |
| C | -3.06661400 | 0.73452800 | -0.67497200 |
| C | 0.58809300 | -0.53148600 | 1.38364400 |
| C | 1.56884200 | 1.43763800 | 0.04703100 |
| C | 1.03594600 | -0.00853300 | 0.00842900 |
| C | -0.38024900 | 0.16551300 | 2.13345600 |
| C | -1.70711900 | 1.35983600 | -0.65702200 |
| C | 2.31974800 | 3.41901500 | -1.16383800 |
| C | -4.26897200 | 1.44712700 | -0.62514000 |
| C | 1.78631700 | 2.13086900 | -1.15809100 |
| C | -0.79237300 | -0.29110600 | 3.38508000 |
| H | -1.54416500 | 0.27249500 | 3.94167800 |
| C | -5.47063400 | 0.73467700 | -0.61719100 |
| C | -0.24646200 | -1.46110600 | 3.92568000 |
| C | 1.93037200 | 2.06934800 | 1.24572600 |
| C | 2.47328100 | 3.35957200 | 1.24122700 |
| C | 2.66412100 | 4.04302000 | 0.03983600 |
| H | 1.79645600 | 1.55077900 | 2.19501000 |
| H | -4.24845200 | 2.53763900 | -0.58448700 |
| H | -0.80462300 | 1.09156500 | 1.74262300 |
| H | -6.41991600 | 1.27207600 | -0.56854100 |
| H | 3.07914200 | 5.05278700 | 0.03847400 |
| H | -0.57169000 | -1.82181500 | 4.90341700 |
| H | 2.46673300 | 3.93751800 | -2.11337500 |
| H | 1.54019600 | 1.65047900 | -2.10867400 |
| H | 2.74714100 | 3.82841800 | 2.18874700 |
| O | -1.49900300 | -2.48867500 | -0.62387300 |
| C | -3.06782200 | -0.66988400 | -0.72373400 |
| C | 2.07489000 | -0.93846100 | -0.65455100 |
| C | 1.13139200 | -1.69816900 | 1.94258400 |
| C | -1.71166600 | -1.29439800 | -0.76740200 |
| C | 2.62462600 | -2.99518300 | -1.84311000 |
| C | -4.27160000 | -1.38233200 | -0.72065600 |
| C | 1.68036800 | -2.13735300 | -1.27285400 |
| C | 0.71764000 | -2.15828500 | 3.19872900 |
| H | 1.15653000 | -3.07245700 | 3.60382100 |
| C | -5.47185500 | -0.66997600 | -0.66404300 |
| C | 3.44469300 | -0.63369000 | -0.60979900 |
| C | 4.39024600 | -1.49477600 | -1.17591400 |
| C | 3.98500900 | -2.67639800 | -1.80079700 |
| H | 3.77955300 | 0.28790700 | -0.13236500 |
| H | -4.25347000 | -2.47301800 | -0.75478900 |
| H | 1.88586100 | -2.26156500 | 1.39441600 |
| H | -6.42200800 | -1.20784600 | -0.65128700 |
| H | 4.72265000 | -3.34389200 | -2.25080700 |
| H | 2.29091000 | -3.91879000 | -2.32061400 |
| H | 0.62542900 | -2.42899500 | -1.28104500 |
| H | 5.44954900 | -1.23313100 | -1.13028400 |

**7: P5_O_Si**, E = -1784.039833

| | | | |
|---|---|---|---|
| P | -1.99528100 | -1.71678700 | 0.14745400 |
| O | -0.52007400 | 0.62150300 | -0.08388100 |
| O | -4.73462100 | -2.17775900 | 0.25897800 |
| C | 1.36473900 | -1.23229300 | -1.36218600 |

| | | | |
|---|---|---|---|
| C | 1.48616200 | -0.61970800 | 1.70122100 |
| C | 2.05483600 | 1.62564900 | -0.35661700 |
| C | 2.26013200 | -2.30573700 | -1.18935300 |
| H | 2.77150600 | -2.43850400 | -0.23277600 |
| C | 0.72175200 | -1.09720300 | -2.60981300 |
| H | 0.02153200 | -0.27440800 | -2.77520300 |
| C | -3.85400400 | -1.33989000 | 0.15889100 |
| C | -1.69498200 | -0.01512000 | -0.00688200 |
| C | 1.85157500 | -3.06567600 | -3.45210300 |
| H | 2.03632200 | -3.77751100 | -4.25943000 |
| C | 3.25081400 | 1.58958000 | -1.09928400 |
| H | 3.59970900 | 0.64257100 | -1.51940600 |
| C | -4.09050800 | 0.13731500 | 0.02565700 |
| C | 2.50374300 | -3.21348300 | -2.22494200 |
| H | 3.19975800 | -4.04085200 | -2.07088800 |
| C | 0.95872200 | -2.00568900 | -3.64331700 |
| H | 0.44458900 | -1.88869100 | -4.59959400 |
| C | -2.88874200 | 0.85916600 | -0.07009200 |
| C | 1.10069500 | -1.91456900 | 2.10968900 |
| H | 0.55825700 | -2.56544500 | 1.42041200 |
| C | 1.62922400 | 2.86891700 | 0.15340300 |
| H | 0.70234600 | 2.92963700 | 0.72922800 |
| C | 2.18491000 | 0.18360100 | 2.62568800 |
| H | 2.50975100 | 1.18542900 | 2.33502100 |
| C | 3.99738000 | 2.75066600 | -1.32202600 |
| H | 4.92021700 | 2.70100200 | -1.90395600 |
| C | 2.08625100 | -1.56661800 | 4.29526000 |
| H | 2.31798400 | -1.93348000 | 5.29753800 |
| C | 3.55919500 | 3.97372500 | -0.80621300 |
| H | 4.14000400 | 4.88187900 | -0.98106500 |
| C | 2.48131800 | -0.28242400 | 3.90955100 |
| H | 3.02494100 | 0.35703700 | 4.60833300 |
| C | 1.39590700 | -2.38194700 | 3.39286300 |
| H | 1.08409600 | -3.38572900 | 3.68913700 |
| C | 2.37184400 | 4.03172900 | -0.06898000 |
| H | 2.02366800 | 4.98577000 | 0.33306500 |
| C | -2.91214600 | 2.24714500 | -0.21002100 |
| H | -1.98183100 | 2.81041200 | -0.29381200 |
| C | -5.32163200 | 0.77836200 | -0.01047000 |
| H | -6.24021000 | 0.19327200 | 0.06699400 |
| C | -5.34925900 | 2.17772400 | -0.14707200 |
| H | -6.30568900 | 2.70320900 | -0.17658300 |
| C | -4.15666300 | 2.89963300 | -0.24699800 |
| H | -4.19066300 | 3.98570900 | -0.35556500 |
| Si | 1.09878000 | 0.04524300 | -0.01422500 |

**7: P5_P_Si**, E = -1784. 03026564

| | | | |
|---|---|---|---|
| P | 0.62432500 | 0.02585900 | -1.64073100 |
| O | 1.64827300 | -2.52184600 | -1.10222100 |
| O | 1.61743300 | 2.53712700 | -0.92028500 |
| C | -2.19042000 | -1.40842300 | -0.46426600 |
| C | -1.87540400 | 1.66162900 | -0.15375500 |
| C | -0.27279900 | -0.26366000 | 1.70972900 |
| C | -3.58207900 | -1.21294700 | -0.35996700 |
| H | -3.97318400 | -0.23937700 | -0.05383000 |
| C | -1.72212200 | -2.67272400 | -0.87639700 |
| H | -0.64740300 | -2.85457500 | -0.97490700 |
| C | 1.84106900 | 1.34677500 | -1.06711800 |
| C | 1.85434600 | -1.31892900 | -1.16370000 |
| C | -3.99590300 | -3.49587100 | -1.05513000 |
| H | -4.69430000 | -4.30323000 | -1.28621400 |
| C | -0.54724800 | -1.43037700 | 2.44859900 |
| H | -1.19977700 | -2.19727200 | 2.02512900 |
| C | 3.18594000 | 0.71416100 | -0.88593700 |
| C | -4.47704600 | -2.24714500 | -0.65060700 |
| H | -5.55231800 | -2.07529400 | -0.56481000 |
| C | -2.61784300 | -3.70557100 | -1.16877600 |
| H | -2.23638100 | -4.67729600 | -1.49014300 |
| C | 3.19188700 | -0.68874300 | -0.93572500 |
| C | -2.25260800 | 2.16295300 | -1.41593000 |
| H | -2.00344000 | 1.60262400 | -2.32123900 |
| C | 0.57386300 | 0.70596900 | 2.28771500 |
| H | 0.80410900 | 1.62502900 | 1.74256800 |
| C | -2.21350900 | 2.41447000 | 0.98705800 |
| H | -1.93606600 | 2.05149800 | 1.97946600 |
| C | 0.00288900 | -1.62302500 | 3.72004300 |
| H | -0.22245100 | -2.53550000 | 4.27639300 |
| C | -3.26613000 | 4.10744200 | -0.38896500 |
| H | -3.80084500 | 5.05523800 | -0.48083000 |
| C | 0.83845400 | -0.65113100 | 4.27677000 |
| H | 1.26774600 | -0.80083900 | 5.26979600 |
| C | -2.90299200 | 3.62598500 | 0.87148600 |
| H | -3.15464100 | 4.19518600 | 1.76904300 |
| C | -2.94018900 | 3.37255800 | -1.53389800 |
| H | -3.21870000 | 3.74560100 | -2.52178300 |
| C | 1.12266800 | 0.51537500 | 3.55811200 |
| H | 1.77361400 | 1.27935500 | 3.98885300 |
| C | 4.38151400 | -1.40312800 | -0.76218600 |
| H | 4.36568800 | -2.49381900 | -0.79761000 |
| C | 4.36954800 | 1.42492300 | -0.66478400 |
| H | 4.34418000 | 2.51544500 | -0.62662700 |
| C | 5.55863200 | 0.71119500 | -0.49352300 |
| H | 6.49324500 | 1.24769000 | -0.31737200 |
| C | 5.56438100 | -0.69279800 | -0.54134100 |
| H | 6.50322200 | -1.23245000 | -0.40114100 |
| Si | -1.01258900 | -0.00799500 | -0.00634100 |

**8: P5_O_Ge**, E = -3571.752531

| | | | |
|---|---|---|---|
| P | -2.09330800 | -1.60820700 | -0.12402500 |
| O | -0.63685400 | 0.75655900 | -0.02502700 |
| O | -4.82534000 | -2.09409600 | -0.22849800 |
| C | 1.16224400 | -1.28466200 | 1.48598400 |
| C | 2.10627200 | 1.62508600 | 0.37965200 |
| C | 1.50355200 | -0.74192000 | -1.76320200 |
| C | 1.78967000 | -2.53213500 | 1.33303400 |
| H | 2.21201200 | -2.81993900 | 0.36718100 |
| C | 0.62634500 | -0.93739900 | 2.73853300 |
| H | 0.13433400 | 0.02847800 | 2.87705500 |
| C | -3.94593200 | -1.24915800 | -0.16784600 |
| C | -1.79335000 | 0.10720500 | -0.06697400 |
| C | 1.33038100 | -3.06788400 | 3.65022900 |
| H | 1.39082400 | -3.76287700 | 4.49027100 |
| C | 0.95637900 | -1.95260400 | -2.22691300 |
| H | 0.24911600 | -2.50969500 | -1.60847600 |
| C | -4.19465500 | 0.23263900 | -0.11522100 |
| C | 1.87383900 | -3.41900400 | 2.41133400 |
| H | 2.36031700 | -4.38795000 | 2.28103900 |
| C | 0.70653600 | -1.82618600 | 3.81307900 |
| H | 0.27914200 | -1.55062700 | 4.77940900 |
| C | -3.00130800 | 0.97109300 | -0.05749400 |
| C | 1.78714000 | 2.84335800 | -0.24579100 |
| H | 0.93970200 | 2.90003100 | -0.93284200 |
| C | 2.40079600 | -0.04147000 | -2.58895800 |
| H | 2.84260200 | 0.89666400 | -2.24465500 |
| C | 3.19465800 | 1.58303000 | 1.26698000 |
| H | 3.45379500 | 0.64845900 | 1.77151300 |
| C | 1.29607000 | -2.44385100 | -3.49092800 |
| H | 0.85932400 | -3.38137300 | -3.84134400 |
| C | 3.62326900 | 3.93800900 | 0.89631100 |
| H | 4.21070800 | 4.83631200 | 1.09740000 |
| C | 2.18668700 | -1.73674200 | -4.30487000 |
| H | 2.44934600 | -2.12260400 | -5.29214500 |
| C | 3.94989900 | 2.73236800 | 1.52357000 |
| H | 4.79223800 | 2.68579200 | 2.21705100 |

| | | | |
|---|---|---|---|
| C | 2.54025400 | 3.99267800 | 0.01269100 |
| H | 2.28012400 | 4.93413600 | -0.47606800 |
| C | 2.73967500 | -0.53533800 | -3.85248800 |
| H | 3.43689900 | 0.01989100 | -4.48354200 |
| C | -3.03826300 | 2.36427200 | 0.00347600 |
| H | -2.11278300 | 2.93933300 | 0.05394700 |
| C | -5.43234400 | 0.86261000 | -0.11534200 |
| H | -6.34464800 | 0.26445000 | -0.16103400 |
| C | -5.47405600 | 2.26684100 | -0.05628300 |
| H | -6.43585500 | 2.78351300 | -0.05649200 |
| C | -4.28897600 | 3.00566300 | 0.00326900 |
| H | -4.33428500 | 4.09580500 | 0.05038700 |
| Ge | 1.08767300 | -0.00666800 | 0.00640400 |

**8: P5_P_Ge**, E = -3571.76106043

| | | | |
|---|---|---|---|
| Ge | -0.93408300 | -0.00586300 | -0.02123500 |
| P | 0.73591200 | 0.02691900 | -1.72662100 |
| O | 1.73699500 | -2.51126900 | -1.11545100 |
| O | 1.70940200 | 2.54102800 | -0.99273700 |
| C | -2.14871900 | -1.49774400 | -0.45178500 |
| C | -1.87582700 | 1.71682000 | -0.17030200 |
| C | -0.13324400 | -0.23612700 | 1.76506500 |
| C | -3.53716800 | -1.30472200 | -0.35058600 |
| H | -3.93561100 | -0.32666400 | -0.06886200 |
| C | -1.66123900 | -2.76098800 | -0.83057500 |
| H | -0.58482500 | -2.93151700 | -0.92666500 |
| C | 1.94037400 | 1.35103600 | -1.13339700 |
| C | 1.95202000 | -1.31100300 | -1.19897000 |
| C | -3.92861400 | -3.60930600 | -0.98783800 |
| H | -4.61929300 | -4.42894900 | -1.19754600 |
| C | -0.38344200 | -1.40331600 | 2.50491300 |
| H | -1.02264900 | -2.18534900 | 2.08835900 |
| C | 3.28259800 | 0.72165700 | -0.92364200 |
| C | -4.42209100 | -2.35541300 | -0.61528000 |
| H | -5.49899400 | -2.19169100 | -0.53376700 |
| C | -2.54881100 | -3.80921000 | -1.09653800 |
| H | -2.15843100 | -4.78531100 | -1.39308400 |
| C | 3.28782400 | -0.68204700 | -0.95769700 |
| C | -2.24867500 | 2.22250700 | -1.42738700 |
| H | -1.98188100 | 1.68056400 | -2.33854800 |
| C | 0.69249800 | 0.75756100 | 2.32156700 |
| H | 0.89935000 | 1.67576100 | 1.76605400 |
| C | -2.22761500 | 2.43902700 | 0.98193400 |
| H | -1.94698200 | 2.06499600 | 1.96953000 |
| C | 0.17766400 | -1.57426900 | 3.77519200 |
| H | -0.02514100 | -2.48708300 | 4.33966900 |
| C | -3.30165200 | 4.13429200 | -0.37593000 |
| H | -3.85225200 | 5.07390000 | -0.45663900 |
| C | 0.99586400 | -0.58036300 | 4.31955400 |
| H | 1.43358800 | -0.71376000 | 5.31116300 |
| C | -2.93728200 | 3.64079100 | 0.87970200 |
| H | -3.20316600 | 4.19251300 | 1.78408600 |
| C | -2.95674200 | 3.42300000 | -1.52993200 |
| H | -3.23580400 | 3.80659500 | -2.51365900 |
| C | 1.25211200 | 0.58637200 | 3.59150500 |
| H | 1.88957700 | 1.36660900 | 4.01325200 |
| C | 4.47368800 | -1.39561200 | -0.75709200 |
| H | 4.45731800 | -2.48663700 | -0.78006100 |
| C | 4.46329300 | 1.43375000 | -0.69131700 |
| H | 4.43869100 | 2.52464000 | -0.66493500 |
| C | 5.64877500 | 0.72072200 | -0.49431800 |
| H | 6.58126400 | 1.25815400 | -0.30994200 |
| C | 5.65376700 | -0.68382200 | -0.52649700 |
| H | 6.58989700 | -1.22257500 | -0.36614400 |

**9: P5_O_NBS**, E = -1159.42068

| | | | |
|---|---|---|---|
| P | -0.07761600 | 1.70091900 | -0.00008500 |
| O | 2.30468300 | -0.51564100 | -2.31114500 |
| O | 0.71973000 | -0.96940600 | -0.00046000 |
| O | 2.30364500 | -0.51593100 | 2.31108000 |
| N | 2.01056800 | -0.44956900 | -0.00009000 |
| C | -1.61731800 | -0.57410100 | -0.00013900 |
| C | -1.99367900 | -1.91814000 | -0.00010700 |
| H | -1.24449500 | -2.71027300 | -0.00016500 |
| C | 2.74041200 | -0.31514800 | -1.20189400 |
| C | 2.73986800 | -0.31525900 | 1.20205300 |
| C | -0.25996300 | -0.00900500 | -0.00019800 |
| C | 4.13595900 | 0.12193800 | -0.77085100 |
| H | 4.33471200 | 1.11232700 | -1.20427100 |
| C | 4.13554700 | 0.12208100 | 0.77167900 |
| H | 4.86499000 | -0.57389400 | 1.20890200 |
| C | -3.36411900 | -2.22872000 | 0.00000100 |
| H | -3.67498400 | -3.27520100 | 0.00004400 |
| O | -2.60944800 | 2.85458400 | 0.00006000 |
| C | -2.59416600 | 0.43876600 | -0.00006000 |
| C | -3.94819300 | 0.13186000 | 0.00004300 |
| H | -4.68662300 | 0.93585900 | 0.00008500 |
| C | -1.98593200 | 1.80995700 | -0.00002500 |
| H | 4.86543100 | -0.57437200 | -1.20750700 |
| H | 4.33375800 | 1.11264900 | 1.20495300 |
| C | -4.33186100 | -1.22048700 | 0.00006900 |
| H | -5.39073900 | -1.48520600 | 0.00016200 |

**9: P5_P_NBS**, E = -1159.50795662

| | | | |
|---|---|---|---|
| P | -1.20736400 | -0.43879200 | 0.00000000 |
| O | -1.87756700 | -3.44355200 | 0.00000000 |
| O | -0.14574600 | 0.33857200 | 2.47267300 |
| O | 1.90625700 | -0.80559700 | 0.00000000 |
| N | -0.17417400 | -1.84931000 | 0.00000000 |
| C | -0.15269500 | 1.98887800 | 0.70448600 |
| C | 0.07476400 | 3.17172000 | 1.41661500 |
| H | 0.08182300 | 3.15352100 | 2.50773300 |
| C | -0.69743600 | -3.16963900 | 0.00000000 |
| C | 1.24125700 | -1.82111000 | 0.00000000 |
| C | -0.37669200 | 0.65012800 | 1.32110200 |
| C | 0.48254600 | -4.13664100 | 0.00000000 |
| H | 0.39684900 | -4.78585400 | -0.88295900 |
| C | 1.74222700 | -3.25991700 | 0.00000000 |
| H | 2.38077300 | -3.40329300 | 0.88335400 |
| C | 0.29912800 | 4.35033600 | 0.70303800 |
| H | 0.48380000 | 5.28272000 | 1.24030500 |
| O | -0.14574600 | 0.33857200 | -2.47267300 |
| C | -0.15269500 | 1.98887800 | -0.70448600 |
| C | 0.07476400 | 3.17172000 | -1.41661500 |
| H | 0.08182300 | 3.15352100 | -2.50773300 |
| C | -0.37669200 | 0.65012800 | -1.32110200 |
| H | 0.39684900 | -4.78585400 | 0.88295900 |
| H | 2.38077300 | -3.40329300 | -0.88335400 |
| C | 0.29912800 | 4.35033600 | -0.70303800 |
| H | 0.48380000 | 5.28272000 | -1.24030500 |

**10: P5_O_P5**, E = -1598.55780599

| | | | |
|---|---|---|---|
| P | 0.99821600 | -0.76840300 | -0.39357900 |
| P | -1.97142100 | -1.98056900 | -0.46644700 |
| O | 1.85742400 | 1.19910400 | -2.19529100 |
| O | 1.69734000 | -0.63854300 | 2.32011300 |
| C | 3.47870500 | 0.33556800 | -0.61661400 |
| O | -4.74508900 | -2.26016500 | -0.41092600 |
| C | -3.93650400 | -0.02873800 | 0.03426800 |
| O | -0.33682300 | 0.22520700 | -0.07096100 |
| C | -2.68279500 | 0.60450700 | 0.11504100 |
| C | 2.14098800 | 0.47577600 | -1.26089400 |
| C | -1.57636700 | -0.33302200 | -0.13482200 |

| | | | |
|---|---|---|---|
| C | -3.81178000 | -1.48981500 | -0.28556400 |
| C | 4.69919400 | 0.71220900 | -1.18974100 |
| C | -2.59836700 | 1.96779100 | 0.40116600 |
| C | 5.82101300 | 0.01569800 | 0.85801300 |
| C | 3.43266400 | -0.19772800 | 0.68872200 |
| C | -3.78933000 | 2.68476600 | 0.60624700 |
| C | -5.03308200 | 2.05220200 | 0.52585800 |
| C | -5.11415700 | 0.67873200 | 0.23553000 |
| C | 5.86688300 | 0.54871600 | -0.44315400 |
| C | 2.05551600 | -0.51405100 | 1.16607100 |
| C | 4.60683200 | -0.36134100 | 1.43345600 |
| H | 4.71877800 | 1.13164600 | -2.19699900 |
| H | -6.07503000 | 0.16517100 | 0.16664500 |
| H | -5.94597400 | 2.62790900 | 0.68907100 |
| H | -1.62938600 | 2.46397000 | 0.46303300 |
| H | 6.74716900 | -0.09571900 | 1.42522900 |
| H | 6.82799700 | 0.84380100 | -0.86867600 |
| H | -3.74020000 | 3.75187900 | 0.83171600 |
| H | 4.55542800 | -0.76652300 | 2.44540200 |

**10: P5_P_P5**, E = -1598.58322914

| | | | |
|---|---|---|---|
| P | 0.85602100 | -1.41924300 | -0.68721400 |
| P | -0.85617200 | -1.41973000 | 0.68719500 |
| O | 0.49161800 | 1.18217600 | -1.65233300 |
| O | 2.55271300 | -2.28597400 | 1.36532200 |
| C | 2.63170600 | 0.68270700 | -0.65754900 |
| O | -2.55263800 | -2.28574200 | -1.36586900 |
| C | -3.20374500 | -0.28459000 | -0.18990300 |
| O | -0.49186400 | 1.18135900 | 1.65325800 |
| C | -2.63173900 | 0.68243300 | 0.65776400 |
| C | 1.23152200 | 0.39951800 | -1.08761900 |
| C | -1.23171500 | 0.39896100 | 1.08811600 |
| C | -2.32216700 | -1.44492300 | -0.51868600 |
| C | 3.35258600 | 1.82506500 | -1.02306300 |
| C | -3.35261100 | 1.82475500 | 1.02341700 |
| C | 5.21960200 | 1.02100700 | 0.31734300 |
| C | 3.20383500 | -0.28462100 | 0.18968100 |
| C | -4.64836300 | 1.98671700 | 0.52938100 |
| C | -5.21934100 | 1.02128800 | -0.31774600 |
| C | -4.50259500 | -0.12007700 | -0.68277900 |
| C | 4.64849000 | 1.98675600 | -0.52932200 |
| C | 2.32217700 | -1.44492200 | 0.51838600 |
| C | 4.50284100 | -0.12039700 | 0.68223700 |
| H | 2.89112900 | 2.56872100 | -1.67483100 |
| H | -4.92783900 | -0.87690700 | -1.34403000 |
| H | -6.23224800 | 1.17007800 | -0.69707400 |
| H | -2.89125800 | 2.56817600 | 1.67553200 |
| H | 6.23263100 | 1.16956900 | 0.69643400 |
| H | 5.22402000 | 2.87493700 | -0.79755700 |
| H | -5.22389100 | 2.87486200 | 0.79774100 |
| H | 4.92820100 | -0.87747200 | 1.34312600 |

**11: P5_O_PPh2**, E = -1604.134809

| | | | |
|---|---|---|---|
| P | 1.20368700 | -0.13327400 | -1.04293900 |
| P | -1.78896300 | -1.26642100 | -1.47498000 |
| O | -4.55284600 | -1.60487700 | -1.43891700 |
| O | -0.13692500 | 0.53312000 | -0.16773400 |
| C | 1.83054100 | -2.78044400 | -0.50469900 |
| H | 1.63873000 | -2.90855500 | -1.57281600 |
| C | 1.69758200 | -1.50677200 | 0.07309300 |
| C | -1.36645400 | 0.04197900 | -0.42076800 |
| C | -3.60881400 | -0.96562400 | -1.00772800 |
| C | -2.46716900 | 0.71470900 | 0.29692100 |
| C | -3.72089100 | 0.16555600 | -0.02487400 |
| C | 2.19415700 | -3.87899500 | 0.28062800 |
| H | 2.29777300 | -4.86498500 | -0.17630600 |
| C | 2.40943600 | -3.71310600 | 1.65088200 |
| H | 2.68526100 | -4.57081400 | 2.26788500 |
| C | 1.91959600 | -1.34827300 | 1.45337800 |
| H | 1.81768300 | -0.36186300 | 1.91040600 |
| C | 2.39089400 | 1.18654000 | -0.57237700 |
| C | 2.26760400 | -2.44844400 | 2.23729800 |
| H | 2.43320900 | -2.32184900 | 3.30925500 |
| C | 1.99094300 | 2.53432900 | -0.53302600 |
| H | 0.93818700 | 2.79289100 | -0.65891000 |
| C | -4.89032700 | 0.66449400 | 0.53294900 |
| H | -5.85113000 | 0.22139900 | 0.26344600 |
| C | -4.80171600 | 1.73571000 | 1.43952900 |
| H | -5.70803200 | 2.14180800 | 1.89270800 |
| C | -2.37493100 | 1.77738400 | 1.19693600 |
| H | -1.40474500 | 2.20461900 | 1.45383700 |
| C | 4.28616700 | 3.22906800 | -0.17097600 |
| H | 5.02009600 | 4.02143100 | -0.01192100 |
| C | -3.55723400 | 2.28230800 | 1.76504500 |
| H | -3.50092700 | 3.11364000 | 2.47080400 |
| C | 2.93223300 | 3.54505900 | -0.32170200 |
| H | 2.60515700 | 4.58618400 | -0.28000200 |
| C | 4.69465200 | 1.89310200 | -0.22646500 |
| H | 5.74945200 | 1.63671800 | -0.10795700 |
| C | 3.75536900 | 0.87825300 | -0.42464900 |
| H | 4.08677800 | -0.16214400 | -0.45481900 |

**11: P5_P_PPh2**, E = -1604.14838572

| | | | |
|---|---|---|---|
| P | 1.24481800 | -0.02230300 | -1.27939700 |
| P | -0.20983000 | -1.56209600 | -0.56642700 |
| O | -1.89678000 | -0.93004600 | -2.70310200 |
| O | -0.43770700 | -0.85364100 | 2.12741900 |
| C | 3.97199500 | -0.39269000 | -1.05039700 |
| H | 3.96945700 | 0.01158100 | -2.06576200 |
| C | 2.75482900 | -0.54289900 | -0.36062400 |
| C | -1.00204400 | -1.00597300 | 1.05487400 |
| C | -1.77225000 | -1.05447800 | -1.49689100 |
| C | -2.47218000 | -0.84980500 | 0.83911800 |
| C | -2.87960100 | -0.88321600 | -0.50611400 |
| C | 5.17958100 | -0.76659600 | -0.45410300 |
| H | 6.11597600 | -0.64431900 | -1.00225900 |
| C | 5.18382800 | -1.30827500 | 0.83426400 |
| H | 6.12509600 | -1.61104400 | 1.29763300 |
| C | 2.77001000 | -1.08435300 | 0.93826000 |
| H | 1.83593700 | -1.19681100 | 1.49610600 |
| C | 0.72585100 | 1.54927800 | -0.46353600 |
| C | 3.97881000 | -1.46720900 | 1.52681300 |
| H | 3.97729500 | -1.89134000 | 2.53314200 |
| C | -0.24637900 | 2.30622200 | -1.14753600 |
| H | -0.65898000 | 1.93149700 | -2.08799300 |
| C | -4.22922800 | -0.74289700 | -0.84531300 |
| H | -4.52636100 | -0.76755400 | -1.89528900 |
| C | -5.16412000 | -0.56805100 | 0.17769800 |
| H | -6.22189600 | -0.45289000 | -0.06749000 |
| C | -3.40986700 | -0.67492900 | 1.86287000 |
| H | -3.07560200 | -0.64667100 | 2.90143500 |
| C | -0.12828200 | 4.03292500 | 0.54580900 |
| H | -0.45613400 | 4.99777500 | 0.93791300 |
| C | -4.75719800 | -0.53402600 | 1.52238600 |
| H | -5.50312700 | -0.39167800 | 2.30700600 |
| C | -0.67678500 | 3.53348100 | -0.64060200 |
| H | -1.43213000 | 4.10777700 | -1.18109400 |
| C | 0.84819500 | 3.29594600 | 1.22205900 |
| H | 1.28298200 | 3.68233100 | 2.14641800 |
| C | 1.27239400 | 2.05974700 | 0.72564700 |
| H | 2.03321800 | 1.49361500 | 1.26497500 |

**13: P5_O_PNR2**, E = -2263.651498

| | | | |
|---|---|---|---|
| P | -0.65151400 | -0.08003500 | 0.25364000 |
| P | 1.72992200 | -0.22781900 | 2.51236500 |
| O | 1.06613100 | 0.30940600 | -0.13969000 |
| N | -1.38144300 | 1.08072300 | -0.75131400 |
| N | -1.00377000 | -1.31089200 | -0.85305800 |
| C | 0.27183400 | -3.42383900 | -1.07833000 |
| C | -1.69274400 | 2.42391300 | -0.33687100 |
| O | 4.15084000 | -0.10989700 | 3.86792100 |
| C | 4.25844300 | 0.46944900 | 1.52889100 |
| C | -1.89267500 | -3.40240800 | 0.10451400 |
| C | -2.30079100 | 5.05890600 | 0.40765000 |
| H | -2.53481800 | 6.08436000 | 0.70132500 |
| C | 3.81560400 | 0.93885900 | -0.81133200 |
| H | 3.12157700 | 1.01163000 | -1.64938800 |
| C | -0.86304500 | -2.72260400 | -0.59673100 |
| C | -1.75553200 | -4.78178900 | 0.31805400 |
| H | -2.53512200 | -5.31630000 | 0.86555800 |
| C | -0.99694700 | 3.50402800 | -0.94054000 |
| C | -2.70120800 | 2.66414900 | 0.63216400 |
| C | 1.97130600 | 0.22487300 | 0.84437100 |
| C | 0.34633200 | -4.80613700 | -0.85557700 |
| H | 1.21325900 | -5.35926600 | -1.22346700 |
| C | 6.07160300 | 1.12850900 | 0.09407900 |
| H | 7.12972300 | 1.35137500 | -0.05685200 |
| C | 0.08827300 | 3.29234700 | -1.98946100 |
| H | 0.25529100 | 2.20800000 | -2.07235400 |
| C | -0.65238300 | -5.48388300 | -0.16040800 |
| H | -0.56895100 | -6.55907900 | 0.01147900 |
| C | -1.32579800 | 4.81105800 | -0.55621000 |
| H | -0.79809100 | 5.65110800 | -1.01349400 |
| C | 5.60865700 | 0.74878500 | 1.36647600 |
| H | 6.28403000 | 0.66823000 | 2.22076500 |
| C | 3.57753600 | 0.04269300 | 2.79987900 |
| C | -1.34707600 | -0.82028400 | -2.20452100 |
| H | -2.03381900 | -1.52960400 | -2.68835400 |
| H | -0.44822900 | -0.72343100 | -2.84012300 |
| C | -3.13735300 | -2.70087600 | 0.63352500 |
| H | -3.08686100 | -1.65072100 | 0.30833200 |
| C | 3.35955700 | 0.56364900 | 0.45325600 |
| C | -3.50357200 | 1.54931500 | 1.29238700 |
| H | -3.18935500 | 0.59551800 | 0.83987500 |
| C | 1.40969700 | -2.73654000 | -1.82494200 |
| H | 1.23324400 | -1.65230500 | -1.77849100 |
| C | -3.20912300 | 1.46125800 | 2.80199200 |
| H | -2.13915500 | 1.29437900 | 2.99126800 |
| H | -3.77014100 | 0.63088900 | 3.25719900 |
| H | -3.50418000 | 2.38818200 | 3.31785200 |
| C | 1.42408300 | 3.92949400 | -1.56365400 |
| H | 1.34047500 | 5.02383800 | -1.47717700 |
| H | 2.20518800 | 3.71683200 | -2.30974700 |
| H | 1.76276200 | 3.53885000 | -0.59407200 |
| C | -2.97500300 | 3.99158100 | 0.99472100 |
| H | -3.74022500 | 4.19059000 | 1.74842400 |
| C | 5.18226000 | 1.22032400 | -0.98028600 |
| H | 5.55307400 | 1.51544400 | -1.96421400 |
| C | -0.34917100 | 3.82397800 | -3.36929000 |
| H | -1.29636800 | 3.37222400 | -3.70094000 |
| H | 0.41776800 | 3.60630500 | -4.12886100 |
| H | -0.49571800 | 4.91516200 | -3.34577200 |
| C | -2.00372300 | 0.54143800 | -1.97554400 |
| H | -1.83205500 | 1.21701300 | -2.82816200 |
| H | -3.09687400 | 0.44278000 | -1.83473100 |
| C | -5.01463500 | 1.70359400 | 1.03149200 |
| H | -5.41208900 | 2.61941900 | 1.49520100 |
| H | -5.56546800 | 0.85105100 | 1.45756900 |
| H | -5.23551300 | 1.75185200 | -0.04518200 |
| C | -3.17369600 | -2.71083000 | 2.17373800 |
| H | -3.22499700 | -3.73945800 | 2.56331500 |
| H | -4.05884100 | -2.16984900 | 2.54264700 |
| H | -2.27781100 | -2.23509400 | 2.59772600 |
| C | 2.77266500 | -2.99764100 | -1.15618700 |
| H | 2.76099300 | -2.70256500 | -0.09720900 |
| H | 3.56222100 | -2.42197100 | -1.66226800 |
| H | 3.05285800 | -4.06095400 | -1.20747800 |
| C | 1.44168300 | -3.15617400 | -3.30841800 |
| H | 1.63938700 | -4.23475100 | -3.40969200 |
| H | 2.23828800 | -2.61803200 | -3.84533100 |
| H | 0.48638600 | -2.94627500 | -3.81259400 |
| C | -4.42801000 | -3.30309700 | 0.04564300 |
| H | -4.41741100 | -3.28377600 | -1.05433800 |
| H | -5.30666800 | -2.73603800 | 0.38972300 |
| H | -4.56544600 | -4.34924700 | 0.35952700 |

**13: P5_P_PNR2**, E = -2263.646846

| | | | |
|---|---|---|---|
| P | -0.58393600 | -0.42811900 | 0.41948400 |
| N | -1.85674800 | 0.03599800 | -0.63387400 |
| N | 0.18826500 | -1.28246500 | -0.83528600 |
| C | 2.45836900 | -2.21251500 | -1.13138300 |
| C | -2.98431100 | 0.83475500 | -0.24777400 |
| C | 0.71813900 | -3.55553600 | -0.01203200 |
| C | -5.20594700 | 2.39706200 | 0.46395700 |
| H | -6.06884000 | 3.00574900 | 0.74246000 |
| C | 1.13121300 | -2.35113300 | -0.64429400 |
| C | 1.65769400 | -4.58624200 | 0.13848700 |
| H | 1.35418300 | -5.51209900 | 0.63228900 |
| C | -3.13730000 | 2.13688300 | -0.79997800 |
| C | -3.94773100 | 0.31836300 | 0.65905700 |
| C | 3.34355800 | -3.28890400 | -0.98242000 |
| H | 4.36373700 | -3.19468900 | -1.35991400 |
| C | -2.12999400 | 2.74869000 | -1.76771700 |
| H | -1.25022000 | 2.08733000 | -1.80393200 |
| C | 2.95715200 | -4.46515000 | -0.34474800 |
| H | 3.66747300 | -5.28593600 | -0.22552300 |
| C | -4.26310600 | 2.88789500 | -0.43666400 |
| H | -4.39330100 | 3.88764700 | -0.85660300 |
| C | -0.31064100 | -0.91765100 | -2.17989100 |
| H | -0.17903200 | -1.76896000 | -2.86160300 |
| H | 0.23666000 | -0.04894300 | -2.58573600 |
| C | -0.70175500 | -3.80613600 | 0.48247100 |
| H | -1.30515900 | -2.91753400 | 0.24148800 |
| C | -3.86447600 | -1.08266300 | 1.25388000 |
| H | -2.98223800 | -1.57890100 | 0.82145200 |
| C | 2.95135300 | -0.94424300 | -1.81739800 |
| H | 2.20677200 | -0.15500000 | -1.63890300 |
| C | -3.66597700 | -1.03844000 | 2.78077100 |
| H | -2.75351100 | -0.48725500 | 3.04984000 |
| H | -3.58147100 | -2.05706600 | 3.18937100 |
| H | -4.51700600 | -0.54728000 | 3.27777900 |
| C | -1.63357500 | 4.12757700 | -1.29282600 |
| H | -2.44007300 | 4.87695700 | -1.31197900 |
| H | -0.82729900 | 4.48318900 | -1.95091500 |
| H | -1.23965600 | 4.07612300 | -0.26789300 |
| C | -5.03995000 | 1.12652200 | 1.00768400 |
| H | -5.78269600 | 0.74263300 | 1.71072000 |
| C | -2.71068600 | 2.86098200 | -3.19298500 |
| H | -3.07419800 | 1.89432800 | -3.57359600 |
| H | -1.94743200 | 3.23869500 | -3.89038300 |
| H | -3.56149800 | 3.56005600 | -3.21380000 |
| C | -1.78485100 | -0.57608200 | -1.97157600 |
| H | -2.14435200 | 0.12664300 | -2.73716600 |
| H | -2.41749000 | -1.48357200 | -2.01627400 |
| C | -5.09499000 | -1.93180700 | 0.87955200 |
| H | -6.01817800 | -1.51797300 | 1.31339800 |
| H | -4.98165700 | -2.95867400 | 1.26006300 |
| H | -5.23205300 | -1.98270300 | -0.21077200 |
| C | -0.74772100 | -3.99245200 | 2.01025100 |
| H | -0.16409800 | -4.87260600 | 2.32167000 |
| H | -1.78425700 | -4.14308200 | 2.34919700 |

| | | | |
|---|---|---|---|
| H | -0.34040900 | -3.11391500 | 2.53045300 |
| C | 4.28717100 | -0.44727100 | -1.23517600 |
| H | 4.23097300 | -0.32187400 | -0.14467000 |
| H | 4.55096000 | 0.52447400 | -1.67761300 |
| H | 5.11111800 | -1.14380500 | -1.45362400 |
| C | 3.08059500 | -1.14307800 | -3.34189500 |
| H | 3.84172000 | -1.90537600 | -3.57177800 |
| H | 3.38354800 | -0.20317800 | -3.82803700 |
| H | 2.13492000 | -1.47243000 | -3.79631100 |
| C | -1.34984600 | -5.00178900 | -0.24316400 |
| H | -1.33852400 | -4.86457200 | -1.33466500 |
| H | -2.39632600 | -5.12216100 | 0.07675800 |
| H | -0.82371500 | -5.94244900 | -0.01958600 |
| P | 0.34175100 | 1.73385000 | 0.87747400 |
| C | 1.56520200 | 1.32811300 | 2.22635400 |
| C | 1.72395500 | 2.30675000 | -0.23740200 |
| O | 1.34531700 | 0.69570800 | 3.25085400 |
| C | 2.88464400 | 1.95906800 | 1.88904500 |
| O | 1.65970500 | 2.54738300 | -1.43884600 |
| C | 2.96129100 | 2.49084300 | 0.59063400 |
| C | 3.97241500 | 2.04789800 | 2.75999400 |
| C | 4.12329700 | 3.12965400 | 0.15089900 |
| H | 3.89539000 | 1.62351300 | 3.76279400 |
| C | 5.13749000 | 2.68670600 | 2.31943400 |
| H | 4.16527000 | 3.53861600 | -0.86032200 |
| C | 5.21086000 | 3.22645700 | 1.02642400 |
| H | 5.99778400 | 2.76796600 | 2.98713000 |
| H | 6.12691800 | 3.72393400 | 0.70098100 |

**$13^{M}$: P5_O_PNR2$^{M}$**, E =-1408.7464986

| | | | |
|---|---|---|---|
| P | -2.06693400 | -0.23452100 | -0.79705500 |
| P | 0.76973800 | -1.86826500 | -0.45638700 |
| O | -0.55535700 | 0.53344900 | -0.13874600 |
| N | -2.73493800 | -0.98936400 | 0.54777700 |
| N | -3.07440900 | 1.11443100 | -0.58859400 |
| O | 3.46712000 | -2.53988300 | -0.36193800 |
| C | 2.96801500 | -0.21236000 | 0.03468600 |
| C | 1.94128000 | 1.96447200 | 0.35766900 |
| C | 0.57811900 | -0.16153900 | -0.16108000 |
| C | 4.35982400 | 1.69110300 | 0.50332600 |
| C | 4.23640400 | 0.31644800 | 0.23425900 |
| C | 2.63818600 | -1.64910900 | -0.26698500 |
| C | -3.49660400 | 1.26202100 | 0.81301100 |
| C | 1.82290200 | 0.59986500 | 0.09225200 |
| C | 3.22321700 | 2.50249100 | 0.56385000 |
| C | -3.66815600 | -0.16954600 | 1.32935400 |
| H | -4.70156900 | -0.53169500 | 1.16491000 |
| H | 1.05406100 | 2.59749600 | 0.40295900 |
| H | 3.33171400 | 3.56869700 | 0.77368400 |
| H | -3.45294600 | -0.23864700 | 2.40925100 |
| H | -4.43890400 | 1.83058100 | 0.86562700 |
| H | 5.10996600 | -0.33646100 | 0.18016600 |
| H | 5.34717500 | 2.12761700 | 0.66639600 |
| H | -2.73341400 | 1.80846100 | 1.40185300 |
| C | -2.75317400 | -2.43004600 | 0.75352900 |
| H | -2.40066400 | -2.68702300 | 1.76633200 |
| H | -3.77276000 | -2.83825100 | 0.62442400 |
| H | -2.08303300 | -2.91655300 | 0.03305200 |
| C | -2.85343000 | 2.34212900 | -1.34321100 |
| H | -3.79806200 | 2.90358400 | -1.42310400 |
| H | -2.09519100 | 2.99873100 | -0.87678800 |
| H | -2.51660700 | 2.09569700 | -2.35989100 |

**$13^{M}$: P5_P_PNR2$^{M}$**, E =-1408.7483186

| | | | |
|---|---|---|---|
| P | 1.83318200 | 0.51315400 | 0.90327000 |
| P | 0.21030300 | 0.90862900 | -0.86088400 |
| O | -0.24882100 | -1.77919300 | -1.36306100 |
| N | 1.97780100 | -1.15984200 | 0.98312200 |
| N | 3.27689900 | 0.61537500 | -0.00798700 |
| O | -1.18184400 | 2.73059100 | 0.70378700 |
| C | -2.37977800 | 0.73742200 | 0.06484000 |
| C | -3.13298100 | -1.47283300 | -0.62359600 |
| C | -0.70535700 | -0.70878100 | -0.97244400 |
| C | -4.66696000 | 0.09127400 | 0.43907100 |
| C | -3.65227300 | 1.04916700 | 0.54841700 |
| C | -1.19331300 | 1.65557000 | 0.11941000 |
| C | 3.44306700 | -0.60254400 | -0.81767700 |
| C | -2.12112900 | -0.51530100 | -0.51656500 |
| C | -4.40948900 | -1.15934900 | -0.14293400 |
| C | 2.94936500 | -1.75859000 | 0.06168400 |
| H | 3.77587100 | -2.20892800 | 0.64368600 |
| H | -2.91403800 | -2.44214000 | -1.07548500 |
| H | -5.21375400 | -1.89417400 | -0.21895000 |
| H | 2.47883400 | -2.54613900 | -0.54972900 |
| H | 4.49850400 | -0.72196600 | -1.10931000 |
| H | -3.83232700 | 2.02578000 | 1.00172300 |
| H | -5.66861800 | 0.31649200 | 0.81125700 |
| H | 2.83265200 | -0.53527900 | -1.74290600 |
| C | 1.21849600 | -2.01903800 | 1.87161500 |
| H | 0.55194200 | -2.69612000 | 1.31113700 |
| H | 1.89818200 | -2.63118300 | 2.49170400 |
| H | 0.60384900 | -1.40707500 | 2.54656200 |
| C | 3.62216400 | 1.86992500 | -0.66534700 |
| H | 4.69407600 | 1.86677000 | -0.91726700 |
| H | 3.04167000 | 2.03431400 | -1.59455700 |
| H | 3.43244200 | 2.71144000 | 0.01573100 |

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