Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

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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 **1** were prepared following our recent procedure,[S1] while all other starting materials were purchased from commercial sources. NMR spectra were recorded on Bruker Avance 400 MHz spectrometers (^{1}H, 400.1 MHz; ^{13}C, 100.5 MHz; ^{31}P, 161.9 MHz). All spectra were obtained in the solvent indicated at 25 °C. The chemical shifts (δ) were measured according to IUPAC and expressed in ppm relative to $SiMe_4$ (^{1}H, ^{13}C), and 85% H_3PO_4 (^{31}P). Coupling constants *J* are reported in Hertz [Hz] as absolute values. Because of high sensitivity of these compounds or the contamination of solvents, the elemental analyses gave unsatisfying results with errors larger than 5 %. The high purity of these isolated compounds has been proved mainly by NMR spectra. UV/vis spectra were measured on Shimadzu UV/vis/NIR UV-3600-spectrometer. Melting point (M. P.) were measured on Buchi M-560 apparatus.

Preparation of 2: Phenylacetylene (15.2 mg, 0.15 mmol) in THF (1 mL) was added to a stirred solution of **1** (86.7 mg, 0.1 mmol) in THF (3 mL) at room temperature. After stirring for 1 hour, the solvent was removed under reduced pressure. The remaining solid was washed with acetonitrile, then with hexane and dried *in vacuo* to afford yellowish powder as **2** (79.4 mg, 0.08 mmol, 81.9% yield). Yellowish crystals of **2** were obtained from a saturated hexane and diethyl ether solution via slow evaporation. M. P. = 228 °C (Decomposition). ^{1}H NMR (C_6D_6, 400 MHz): δ = 7.55 (d, *J* = 6.8 Hz, 2 H, $C_{ar}H$), 7.21 (m, 6 H, $C_{ar}H$), 7.10 (m, 9 H, $C_{ar}H$), 5.90 (dd, $^{1}J_{PH}$ = 150.0 Hz, $^{3}J_{PH}$ = 11.6 Hz, 1 H, P*H*), 3.35 (m, 16 H, NCH_2, C*H*Me_2), 1.53 (d, *J* = 6.0 Hz, 6 H, CH_3), 1.40 (m, 18 H, CH_3), 1.23 (d, *J* = 6.0 Hz, 12 H, CH_3), 1.13 (d, *J* = 5.6 Hz, 12 H, CH_3); ^{13}C{^{1}H} NMR (C_6D_6, 100.5 MHz): δ =151.5 (dd, $^{2}J_{PC}$ = 19.2 Hz, $^{2}J_{PC}$ = 16.2 Hz, PC*C*), 150.0 (s, C_{ar}), 149.5 (d, J_{PC} = 4.8 Hz, C_{ar}), 148.7 (d, J_{PC} = 3.8 Hz, C_{ar}), 148.4 (s, C_{ar}), 148.2 (s, C_{ar}), 138.7 (s, C_{ar}), 136.2 (d, J_{PC} = 3.7 Hz, C_{ar}), 131.4 (s, C_{ar}), 128.1 (s, C_{ar}), 128.0 (s, C_{ar}), 127.8 (s, C_{ar}), 126.9 (s, C_{ar}), 126.6 (s, C_{ar}), 124.1 (s, C_{ar}), 123.9 (s, C_{ar}), 123.5 (s, C_{ar}), 123.4 (s, C_{ar}), 103.0 (d, $^{2}J_{PC}$ = 16.6 Hz, PC*C*Ph), 98.5 (d, $^{1}J_{PC}$ = 91.8 Hz, P*C*CPh), 52.1 (s, N*C*H_2), 51.1 (s, N*C*H_2), 48.1 (dd, $^{1}J_{PC}$ = 8.3 Hz, $^{1}J_{PC}$ = 5.1 Hz, P*C*C), 28.5, 28.5, 28.2, 28.0, 25.8, 24.9, 23.7, 23.6, 23.5, 23.2; ^{31}P NMR (C_6D_6, 161.9 MHz) δ = 58.1 (dd, $^{2}J_{PP}$ = 13.4 Hz, $^{3}J_{PH}$ = 11.6 Hz, *P*CPH), 36.2 (dd, $^{2}J_{PP}$ = 13.4 Hz, $^{1}J_{PH}$ = 150.0 Hz, *P*CPH). UV/Vis (CH_2Cl_2, λ (nm) ε ($M^{-1}cm^{-1}$)): 287.3 (23257). IR (ATR, [cm^{-1}]): 2166.6 (PH).

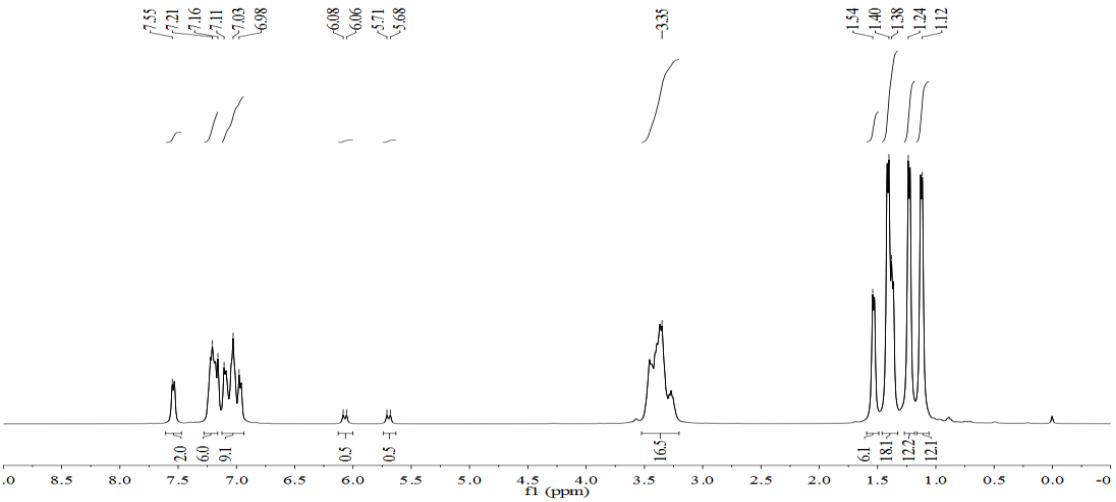

Figure S1. ^{1}H NMR spectrum of **2** in C_6D_6.

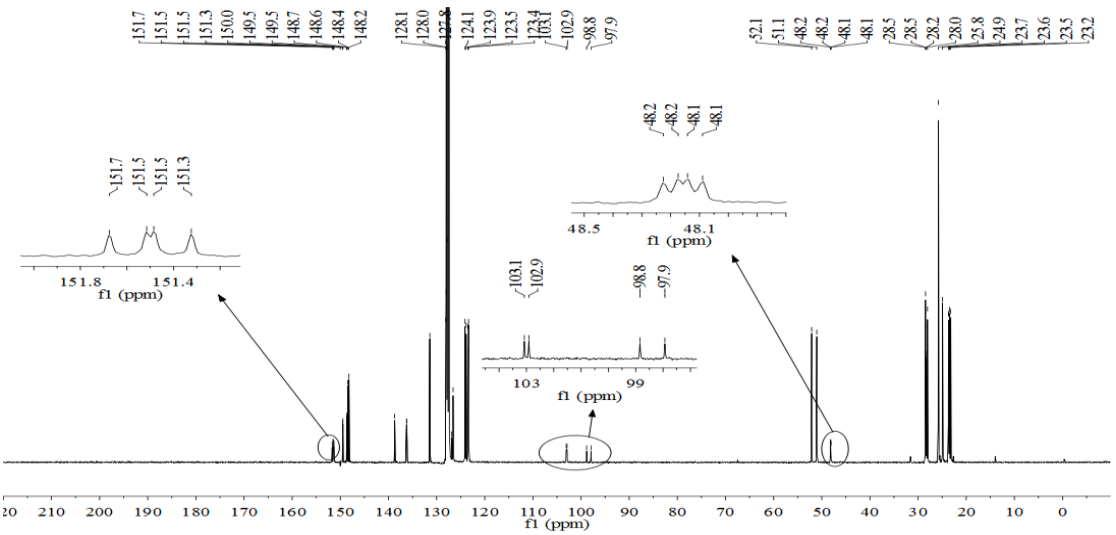

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in C_6D_6.

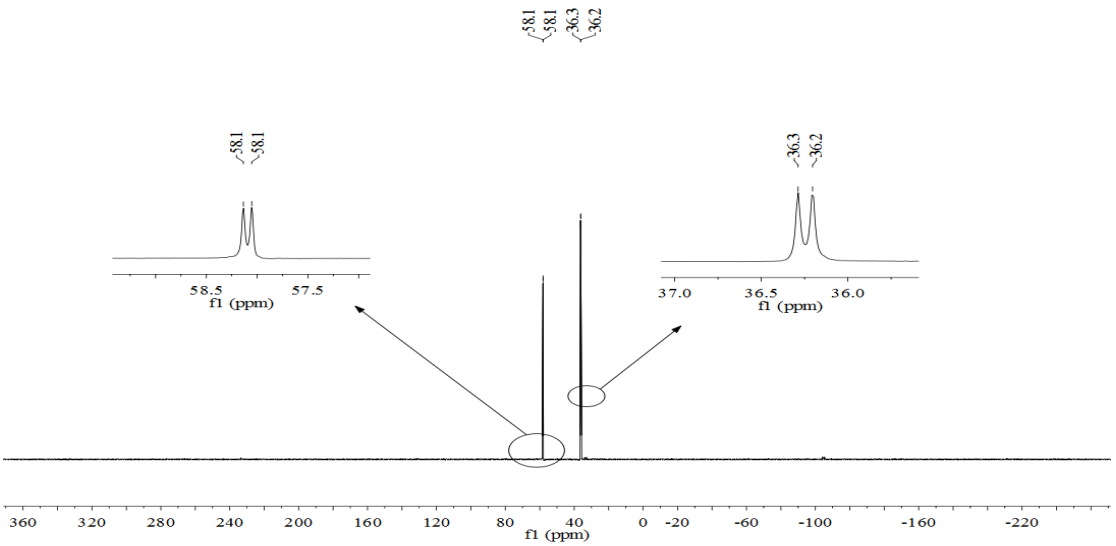

Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of **2** in C_6D_6.

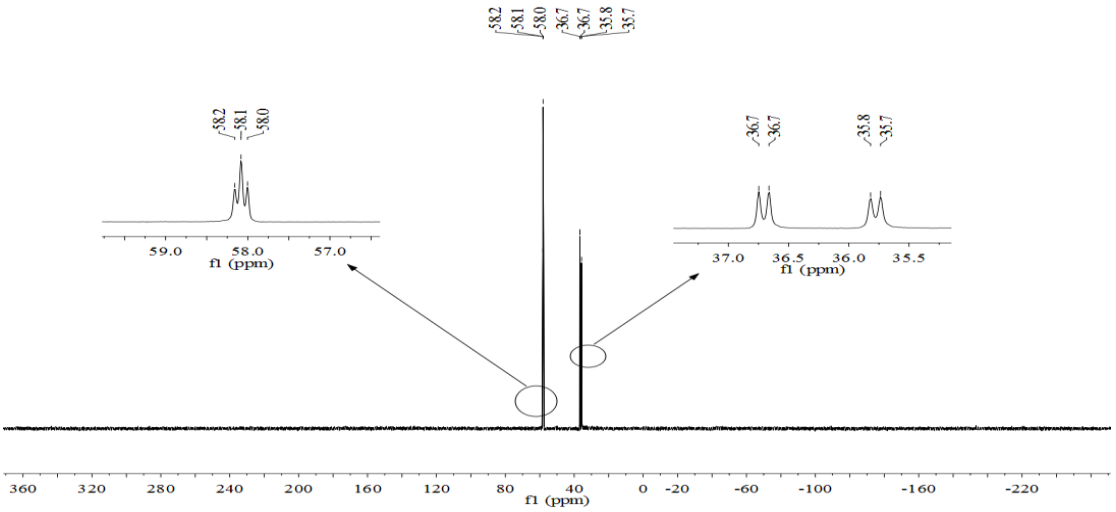

Figure S4. ^{31}P NMR spectrum of **2** in C_6D_6.

Preparation of 3: Malononitrile (6.6 mg, 0.10 mmol) in THF (1 mL) was added dropwise to a stirred solution of **1** (86.8 mg, 0.10 mmol) in THF (4 mL). After stirring for 2 hours at room temperature, the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* to afford **3** as orange powder (0.088 mmol, 87.9% yield). Orange crystals were obtained from a fluorobenzene solution layered with hexane on top and stored at –30 °C. M. P. = 232 °C. ^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 7.38 (m, 4 H, $C_{ar}H$), 7.08 (m, 8 H, $C_{ar}H$), 4.93 (dd, 1 H, $^1J_{PH}$ = 183.2 Hz, P*H*; $^3J_{PH}$ = 21.2 Hz, *P*CP*H*), 4.06 (m, 8 H, CH_2), 2.86 (m, 8 H, C*H*Me$_2$), 1.26 (m, 24 H, CH_3), 1.06 (m, 24 H, CH_3); ^{13}C{^{1}H} NMR (CD_2Cl_2, 100.5 MHz): δ =162.1 (t, $^2J_{PC}$ = 10.2 Hz, PC*C*), 147.3 (C_{ar}), 147.0 (C_{ar}), 132.1 (C_{ar}), 130.7 (C_{ar}), 125.4 (C_{ar}), 125.2 (C_{ar}), 121.8 (dd, $^1J_{PC}$ = 47.4 Hz, $^1J_{PC}$ = 5.4 Hz, P*C*PH), 51.5 (s, N*C*H$_2$), 28.8, 28.8, 25.2, 25.1, 23.3, 23.2; ^{31}P NMR (CD_2Cl_2, 161.9 MHz) δ = 436.2 (dd, $^2J_{PP}$ = 67.7 Hz, $^3J_{PH}$ = 21.2 Hz), 10.2 (dd, $^2J_{PP}$ = 67.7 Hz, $^1J_{PH}$ = 183.2 Hz). UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-1}$): 325.9 (37849), 484.1 (2102). IR (ATR, [cm^{-1}]): 2161.4 (PH).

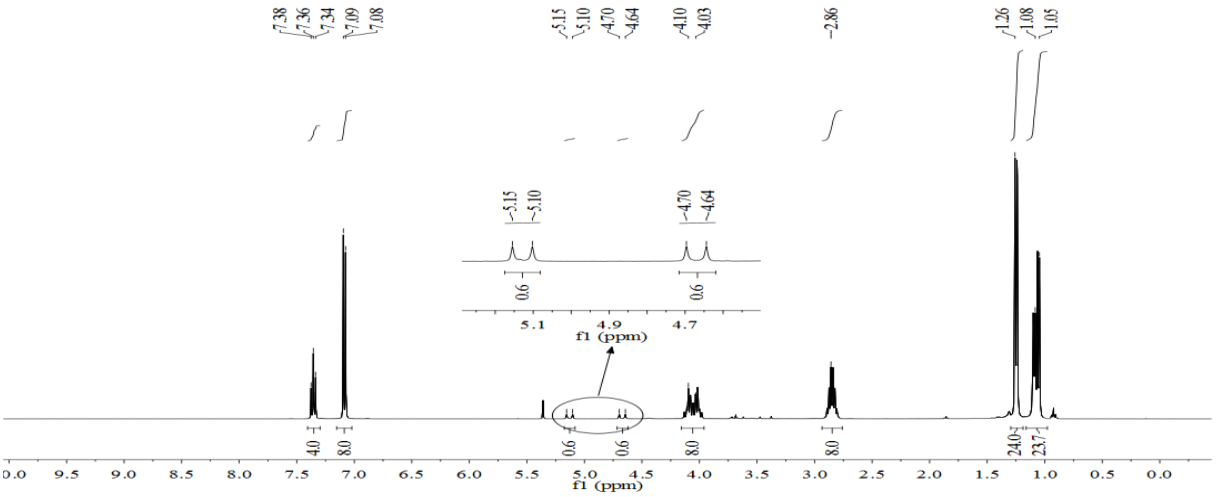

Figure S5. ^{1}H NMR spectrum of **3** in CD_2Cl_2.

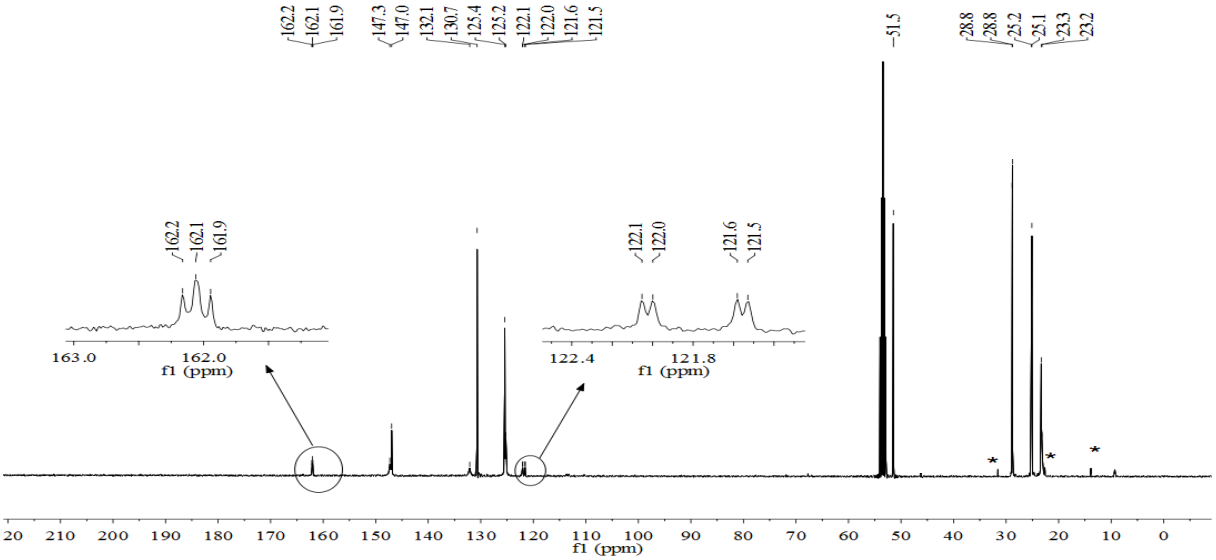

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in CD_2Cl_2. *Hexane.

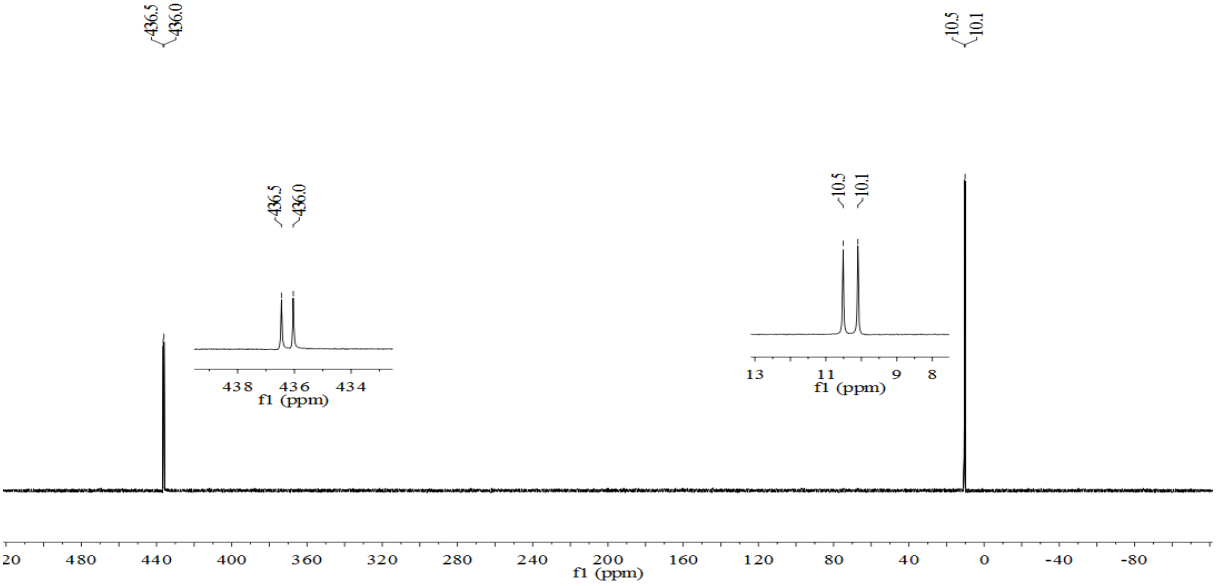

Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in CD_2Cl_2.

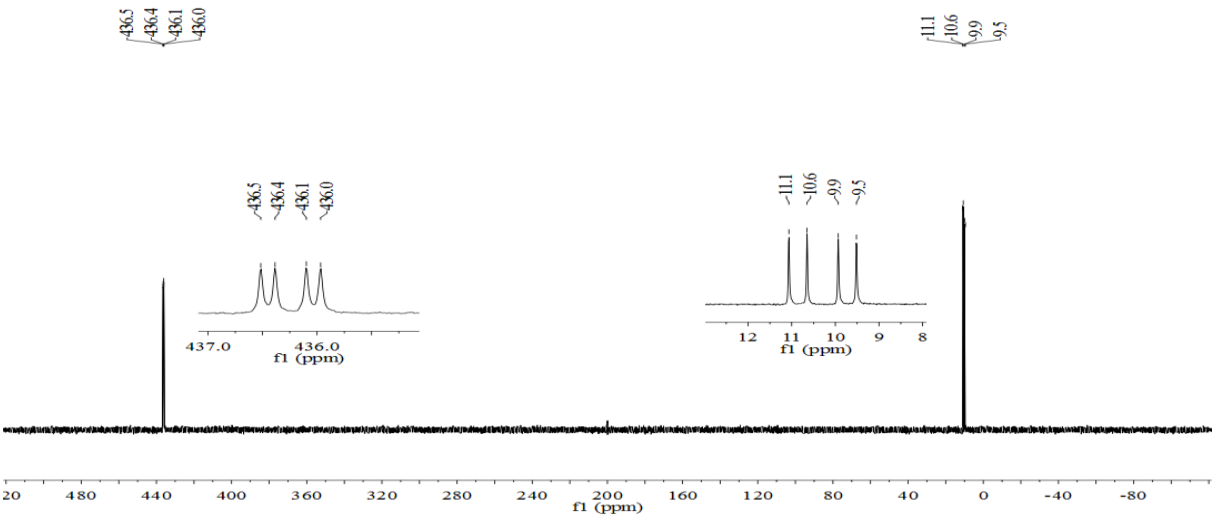

Figure S8. ^{31}P NMR spectrum of **3** in CD_2Cl_2.

Preparation of 4: 2-Iodo-2-methylpropane (92.1 mg, 0.50 mmol) in THF (2 mL) was added dropwise to a stirred solution of **1** (86.8 mg, 0.10 mmol) in THF (4 mL). After stirring for 12 hours at room temperature, the solvent was removed under reduced pressure. The remaining solid was washed with toluene and dried *in vacuo* to afford **4** as orange powder (0.062 mmol, 62.4% yield). M. P. = > 250 °C. ^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 7.35 (m, 4 H, $C_{ar}H$), 7.08 (m, 8 H, $C_{ar}H$), 4.89 (dd, 1 H, $^{1}J_{PH}$ = 182.8 Hz, P*H*; $^{3}J_{PH}$ = 21.0 Hz, *P*CP*H*), 4.05 (m, 8 H, CH_2), 2.85 (m, 8 H, C*H*Me$_2$), 1.12 (m, 48 H, CH_3); ^{13}C{^{1}H} NMR (CD_2Cl_2, 100.5 MHz): δ =162.1 (t, $^{2}J_{PC}$ = 10.8 Hz, PC*C*), 147.3 (C_{ar}), 147.0 (C_{ar}), 132.3 (C_{ar}), 130.7 (C_{ar}), 125.4 (C_{ar}), 125.2 (C_{ar}), 121.8 (dd, $^{1}J_{PC}$ = 47.4 Hz, $^{1}J_{PC}$ = 5.1 Hz, P*C*PH), 51.6 (s, N*C*H$_2$), 28.8, 28.8, 25.2, 25.1, 23.3, 23.2; ^{31}P NMR (CD_2Cl_2, 161.9 MHz) δ = 436.1 (dd, $^{2}J_{PP}$ = 67.5 Hz, $^{3}J_{PH}$ = 21.0 Hz), 10.5 (dd, $^{2}J_{PP}$ = 67.5 Hz, $^{1}J_{PH}$ = 182.8 Hz). UV/Vis (THF, λ (nm) ε ($M^{-1}cm^{-1}$): 320.9 (17004), 481.9 (44461). In the ^{1}H NMR spectrum, the new resonance at 4.74 and 1.35 ppm indicated the formation of isobutene.

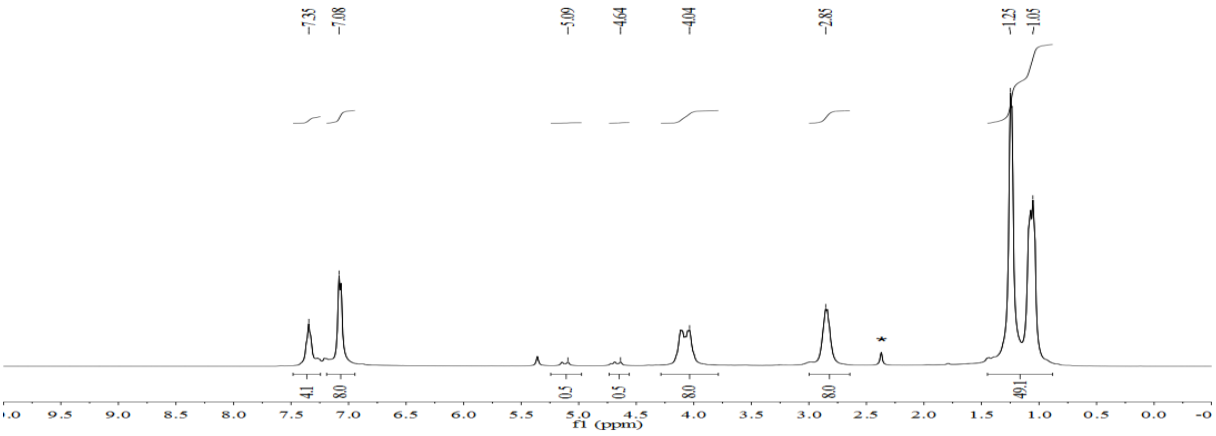

Figure S9. ^{1}H NMR spectrum of **4** in CD_2Cl_2. *Toluene.

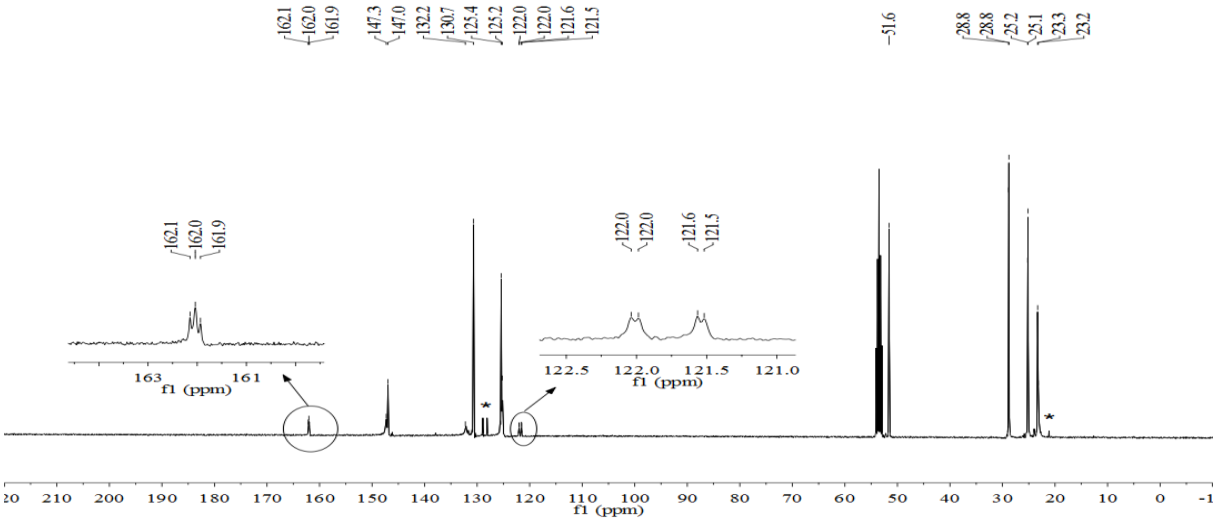

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2. *Toluene.

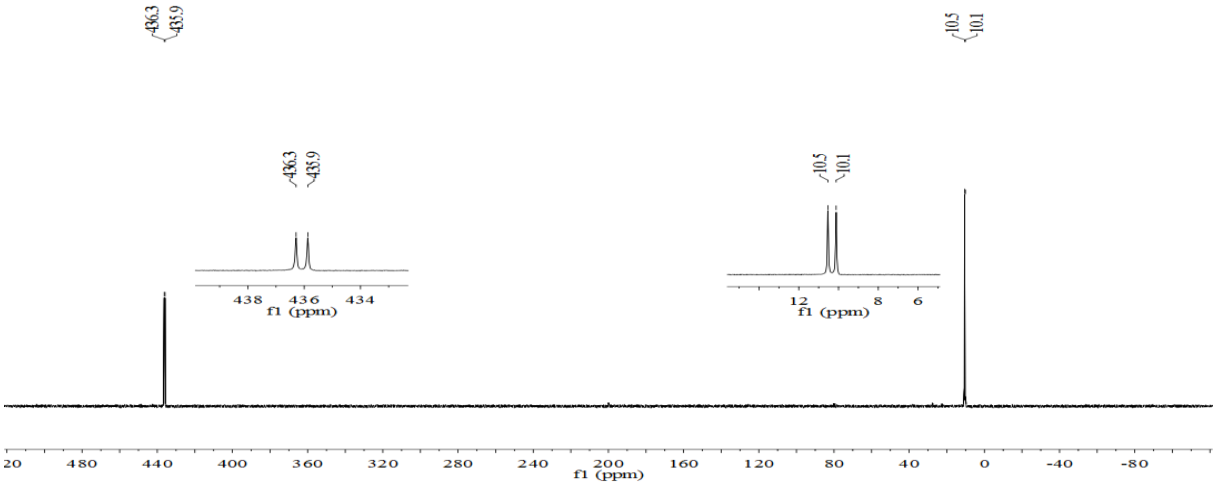

Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2.

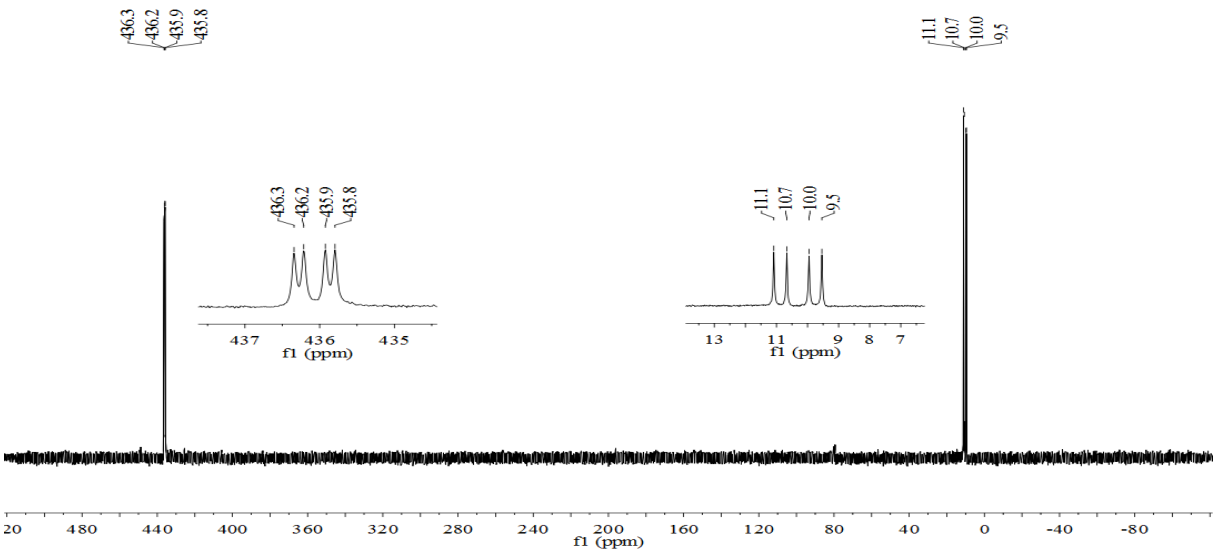

Figure S12. ^{31}P NMR spectrum of **4** in CD_2Cl_2.

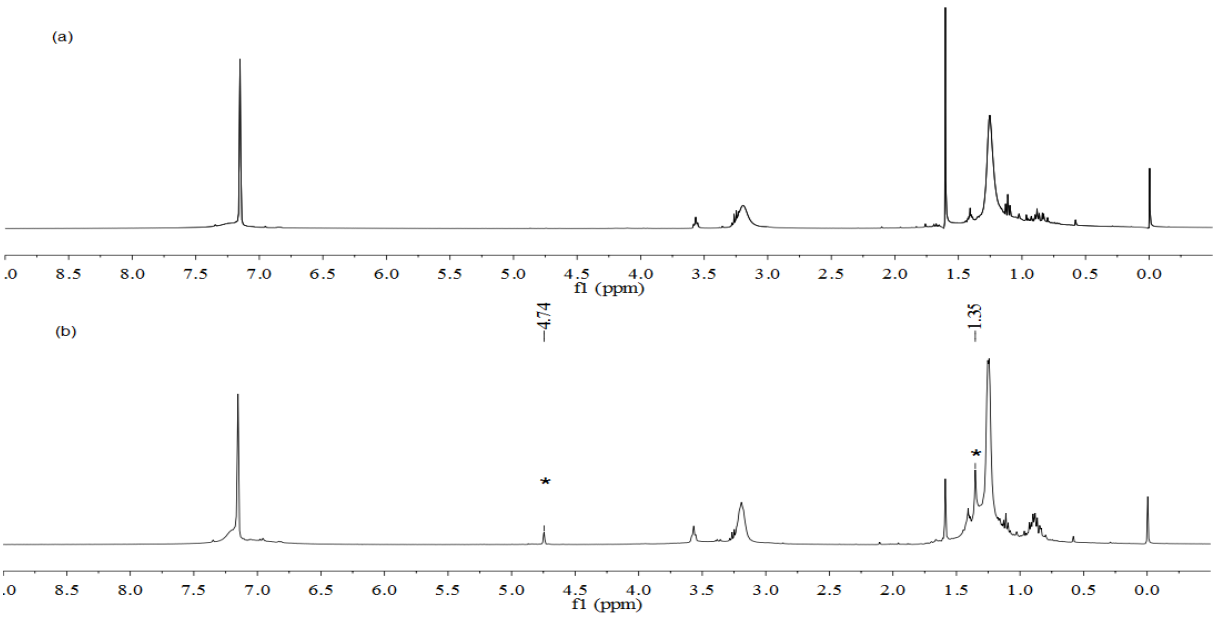

Figure S13. (a) ^{1}H NMR spectrum of **1** and 2-Iodo-2-methylpropane in C_6D_6; (b) After heating the NMR tube at 80 °C for 4 hours. *Indicating the formation of isobutene.

Preparation of 5: $LiAlH_4$ (0.10 mmol) was added to a stirred solution of **3** or **4** (0.10 mmol) in THF (4 mL). After stirring for 0.5 hours, the solvent was removed under reduced pressure. The remaining residue was extracted with toluene and the solvent was removed under reduced pressure. The remaining solid was washed with acetonitrile and dried *in vacuo* to afford **5** as white powder (78.8 mg, 0.09 mmol, 90.7% yield). Only characteristic ^{1}H NMR and ^{31}P NMR data is provided because of the presence of two isomers in the isolated product. ^{1}H NMR (C_6D_6, 400 MHz): *cis*-isomer: δ = 5.59 (d, 1 H, $^{1}J_{PH}$ = 132.4 Hz, P*H*), *trans*-isomer: δ = 4.95 (dd, 1 H, $^{1}J_{PH}$ = 158.4 Hz, *P*CP*H*); ^{31}P NMR (C_6D_6, 161.9 MHz) *cis*-isomer: δ = 33.1 (d, $^{1}J_{PH}$ = 132.4 Hz), *trans*-isomer: δ = 25.8 (d, $^{1}J_{PH}$ = 158.4 Hz). IR (solid): 2168.7 cm^{-1} (b, PH).

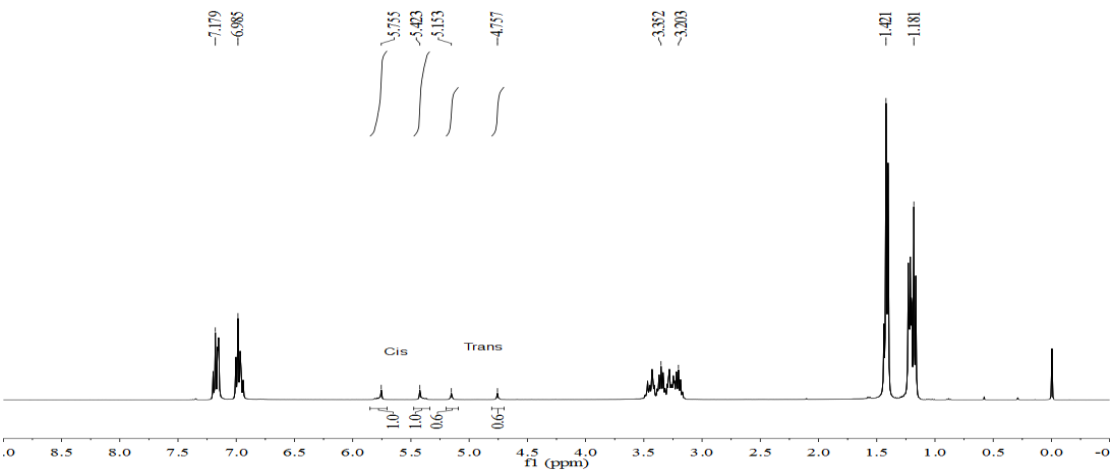

Figure S14. ^{1}H NMR spectrum of **5** in C_6D_6.

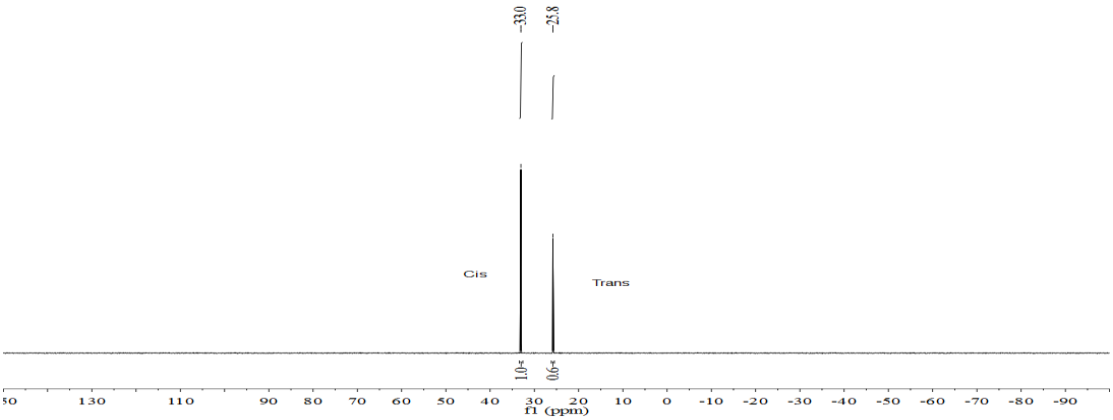

Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of **5** in C_6D_6.

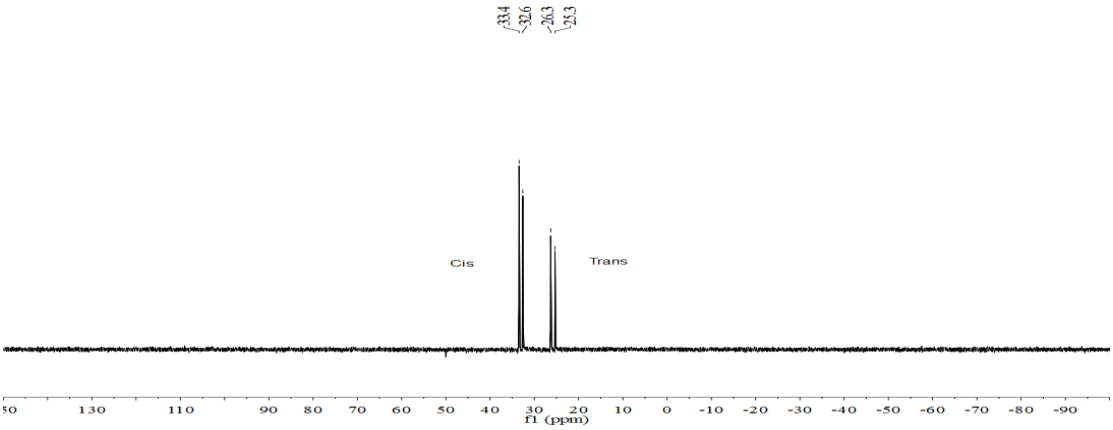

Figure S16. ^{31}P NMR spectrum of **5** in C_6D_6.

Preparation of 6: *p*-CN-aniline (5.0 equivalent) was added to a stirred solution of **1** (86.8 mg, 0.10 mmol) in toluene (10 mL). After stirring for 2 days at 80 °C, the solvent was removed under reduced pressure. The remaining solid was dissolved in the diethyl ether/hexane solution. Yellow crystals were obtained via slow evaporation. The crystals were washed with cold hexane and dried *in vacuo* to afford **6** as yellow crystalline powder (41.5 mg, 0.042 mmol, 42.1% yield). Yellowish crystals suitable for single X-ray diffraction study were obtained from a fluorobenzene solution layered with acetonitrile on top and stored at –30 °C. Only characteristic ^{1}H NMR and ^{31}P NMR data is provided because of the presence of two isomer in the isolated product. ^{1}H NMR (C_6D_6, 400 MHz): *cis*-isomer: δ = 5.49 (dd, 1 H, $^{1}J_{PH}$ = 142.0 Hz, P*H*, $^{3}J_{PH}$ = 9.2 Hz, *P*CP*H*), *trans*-isomer: δ = 4.69 (d, 1 H, $^{1}J_{PH}$ = 155.6 Hz, P*H*); ^{31}P NMR (C_6D_6, 161.9 MHz) *cis*-isomer: δ = 108.5 (m, $^{2}J_{PP}$ = 21.2 Hz), 15.7 (dd, $^{2}J_{PP}$ = 21.2 Hz, $^{1}J_{PH}$ = 142.0 Hz), *trans*-isomer: δ = 108.4 (m, $^{2}J_{PP}$ = 4.0 Hz), 24.5 (d, $^{1}J_{PH}$ = 155.6 Hz).

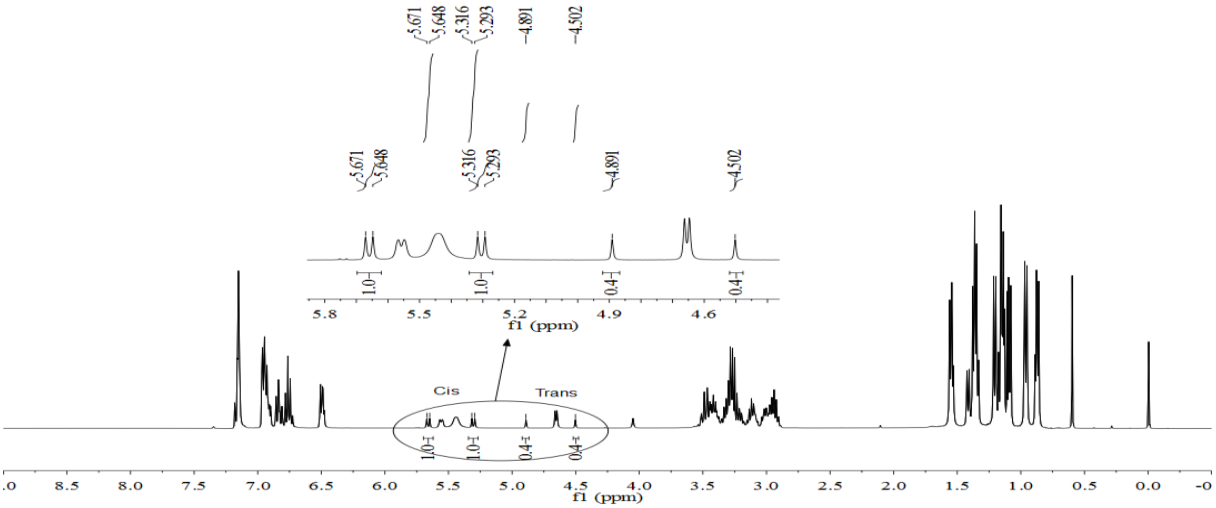

Figure S17. ^{1}H NMR spectrum of **6** in C_6D_6.

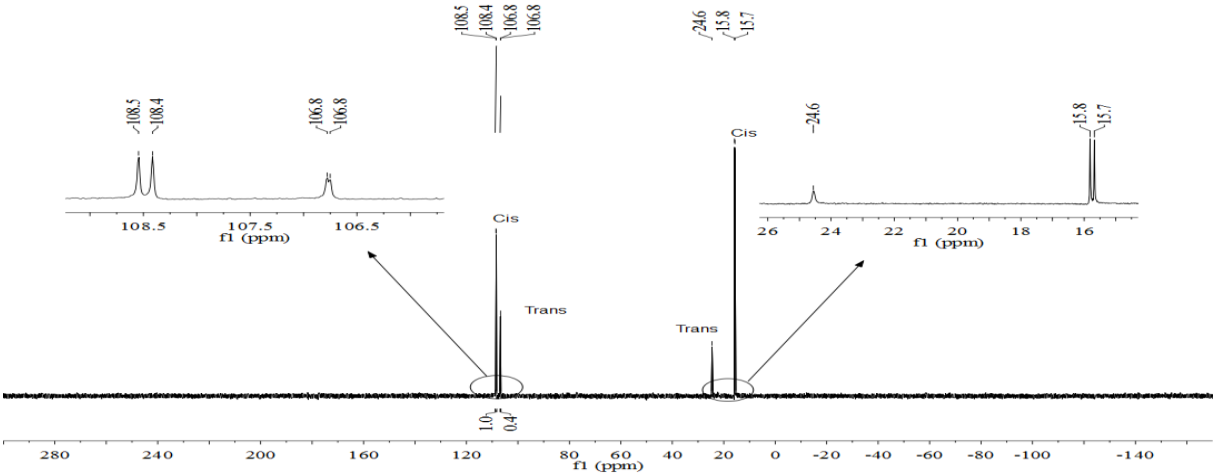

Figure S18. ^{31}P{^{1}H} NMR spectrum of **6** in C_6D_6.

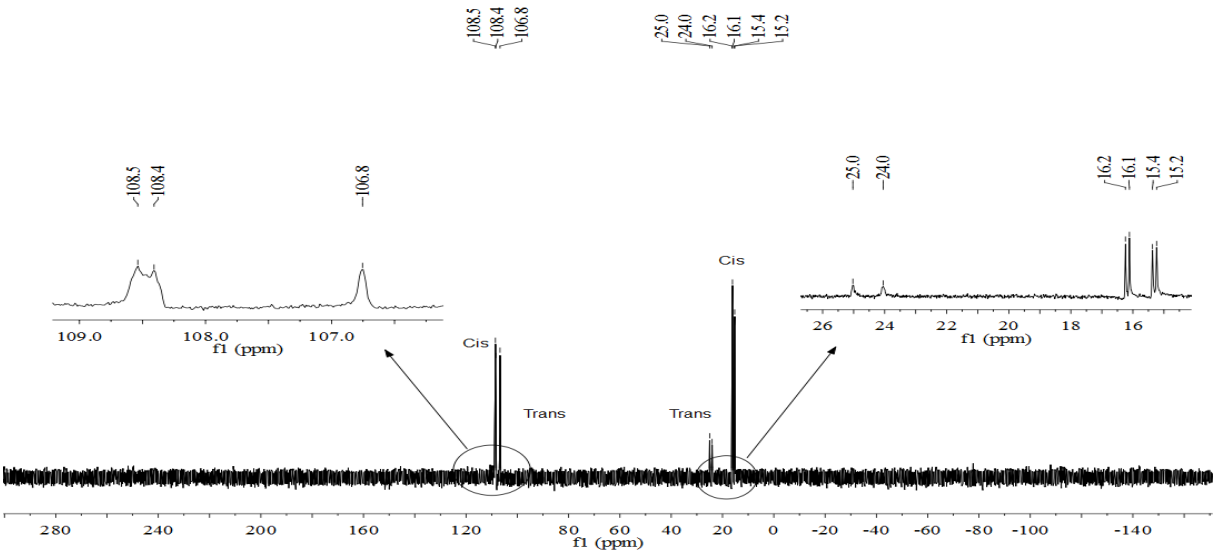

Figure S19. ^{31}P NMR spectrum of **6** in C_6D_6.

Preparation of 7: *p*-CF_3-aniline (5.0 equivalent) was added to a stirred solution of **1** (86.8 mg, 0.10 mmol) in toluene (10 mL). After stirring for 2 days at 80 °C, the solvent was removed under reduced pressure. The remaining solid was dissolved in the diethyl ether/hexane solution. Yellow crystals were obtained via slow evaporation. The crystals were washed with cold hexane and dried *in vacuo* to afford **7** as yellow crystalline powder (48.9 mg, 0.048 mmol, 47.6% yield). Only characteristic ^{1}H NMR and ^{31}P NMR data is provided because of the presence of two isomer in the isolated product. ^{1}H NMR (C_6D_6, 400 MHz): *cis*-isomer: δ = 5.51 (dd, 1 H, $^{1}J_{PH}$ = 142.0 Hz, P*H*, $^{3}J_{PH}$ = 9.6 Hz, *P*CP*H*), *trans*-isomer: δ = 4.70 (d, 1 H, $^{1}J_{PH}$ = 155.6 Hz, P*H*); ^{31}P NMR (C_6D_6, 161.9 MHz) *cis*-isomer: δ = 107.2 (m, $^{2}J_{PP}$ = 20.9 Hz), 14.4 (dd, $^{2}J_{PP}$ = 20.9 Hz, $^{1}J_{PH}$ = 142.0 Hz), *trans*-isomer: δ = 108.4 (m, $^{2}J_{PP}$ = 3.7 Hz), 22.7 (d, $^{1}J_{PH}$ = 155.6 Hz); ^{19}F NMR (C_6D_6) *cis*-isomer: δ = –59.7 (s), *trans*-isomer: δ = –59.8 (s).

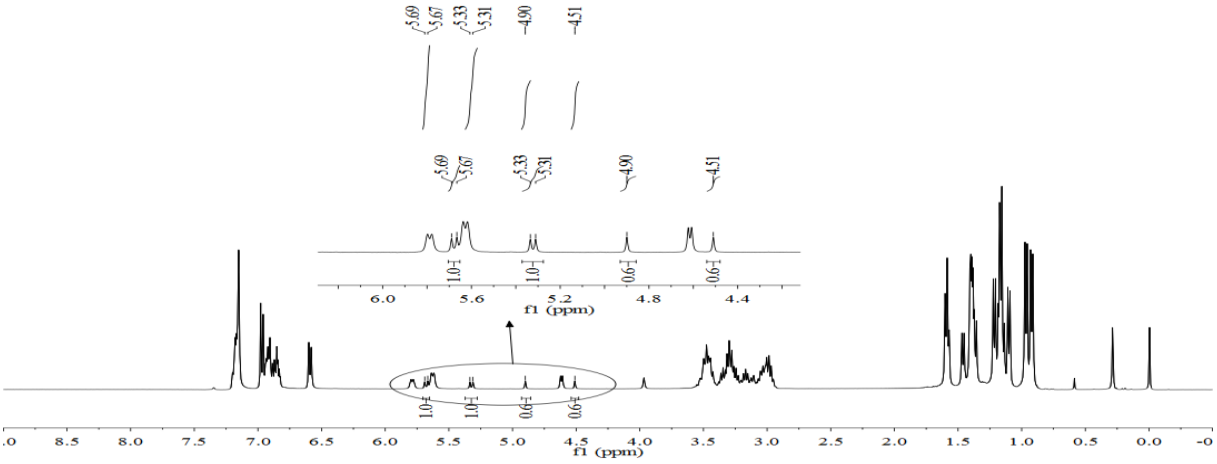

Figure S20. ^{1}H NMR spectrum of **7** in C_6D_6.

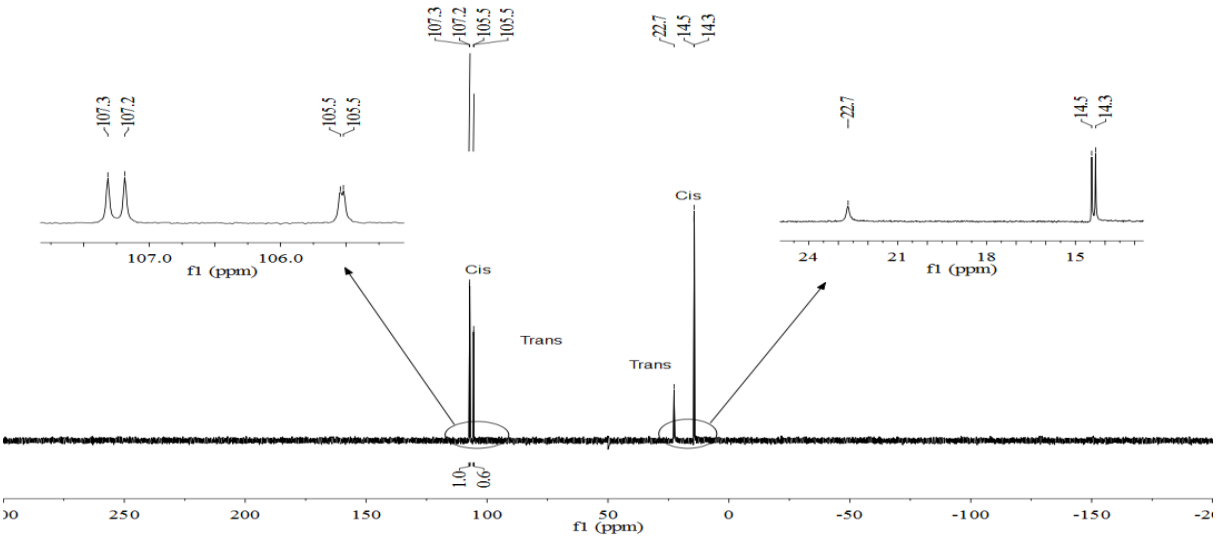

Figure S21. ^{31}P{^{1}H} NMR spectrum of **7** in C_6D_6.

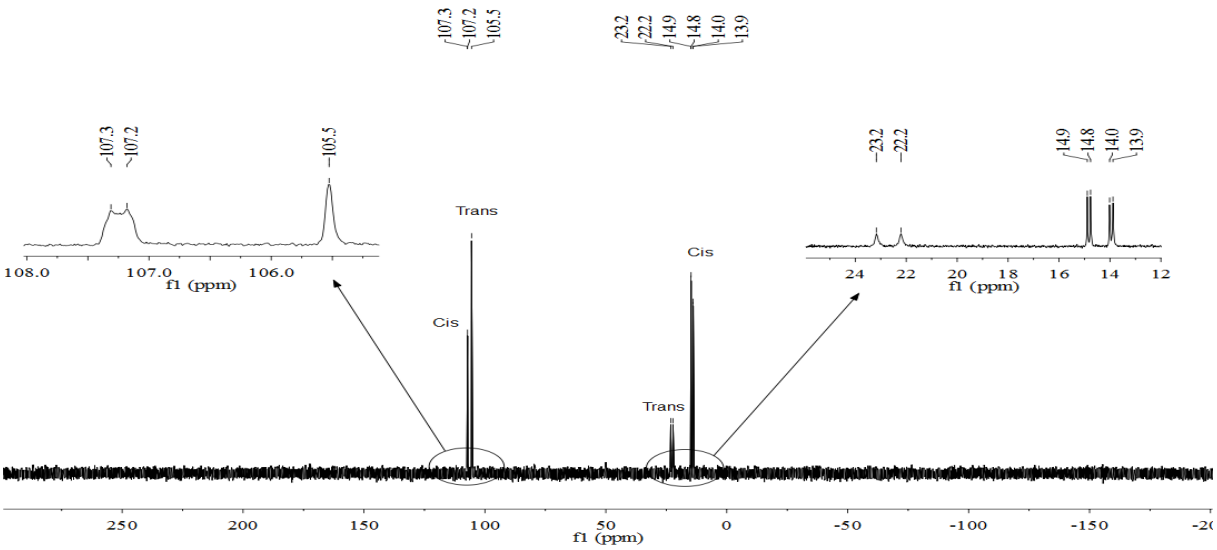

Figure S22. ^{31}P NMR spectrum of **7** in C_6D_6.

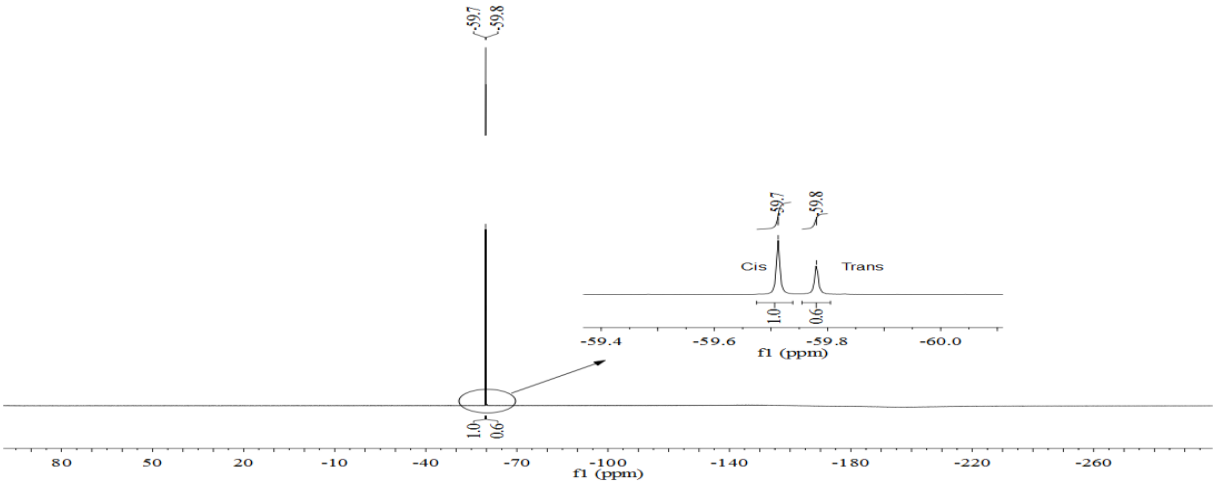

Figure S23. ^{19}F NMR spectrum of **7** in C_6D_6.

Preparation of 9: H_2O (1.0 equivalent) in THF (1 mL) was added to a stirred solution of **1** (86.8 mg, 0.10 mmol) in THF (3 mL). After stirring for 2 hours at 60 °C, the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* to afford **9** as yellowish powder (62.5 mg, 0.071 mmol, 70.6% yield). Yellowish crystals were obtained from a saturated hexane/THF solution via slow evaporation. M. P. = 236 °C. ^{1}H NMR (C_6D_6, 400 MHz): δ = 7.22 (m, 6 H, $C_{ar}H$), 6.93 (m, 6 H, $C_{ar}H$), 5.62 (d, 1 H, $^1J_{PH}$ = 476.5 Hz, P*H*), 3.55 (m, 4 H, C*H*Me$_2$), 3.28 (m, 4 H, C*H*Me$_2$), 3.19 (m, 4 H, NH_2), 3.10 (m, 4 H, NH_2), 1.70 (b, 6 H, CH_3), 1.38 (m, 12 H, CH_3), 1.18 (m, 30 H, CH_3); ^{13}C{^{1}H} NMR (C_6D_6, 100.5 MHz): δ =155.6 (dd, $^2J_{PC}$ = 12.6 Hz, $^2J_{PC}$ = 4.3 Hz, PC*C*), 150.4 (s, C_{ar}), 150.0 (s, C_{ar}), 149.4 (d, J_{PC} = 4.5 Hz, C_{ar}), 149.0 (s, C_{ar}), 147.6 (s, C_{ar}), 147.3 (s, C_{ar}), 147.2 (s, C_{ar}), 147.0 (s, C_{ar}), 136.9 (s, C_{ar}), 135.2 (s, C_{ar}), 135.2 (s, C_{ar}), 128.5 (s, C_{ar}), 128.4 (s, C_{ar}), 127.5 (s, C_{ar}),

124.4 (s, C_{ar}), 123.6 (s, C_{ar}), 123.4 (s, C_{ar}),123.1 (s, C_{ar}), 51.3 (s, N*C*H$_2$), 50.8 (s, N*C*H$_2$), 29.1, 28.5, 28.3, 28.2, 26.4, 25.5, 25.4, 25.4, 24.8, 24.1, 23.4, 23.3, 22.9, 22.7, 22.6; ^{31}P NMR (C_6D_6, 161.9 MHz) δ = 8.0 (dd, $^2J_{PP}$ = 15.4 Hz, $^1J_{PH}$ = 476.5 Hz), –57.8 (dd, $^2J_{PP}$ = 15.4 Hz, $^1J_{PH}$ = 156.7 Hz). IR (solid): 2300.8 (s, P(O)H), 2181.7 cm^{-1} (s, PH).

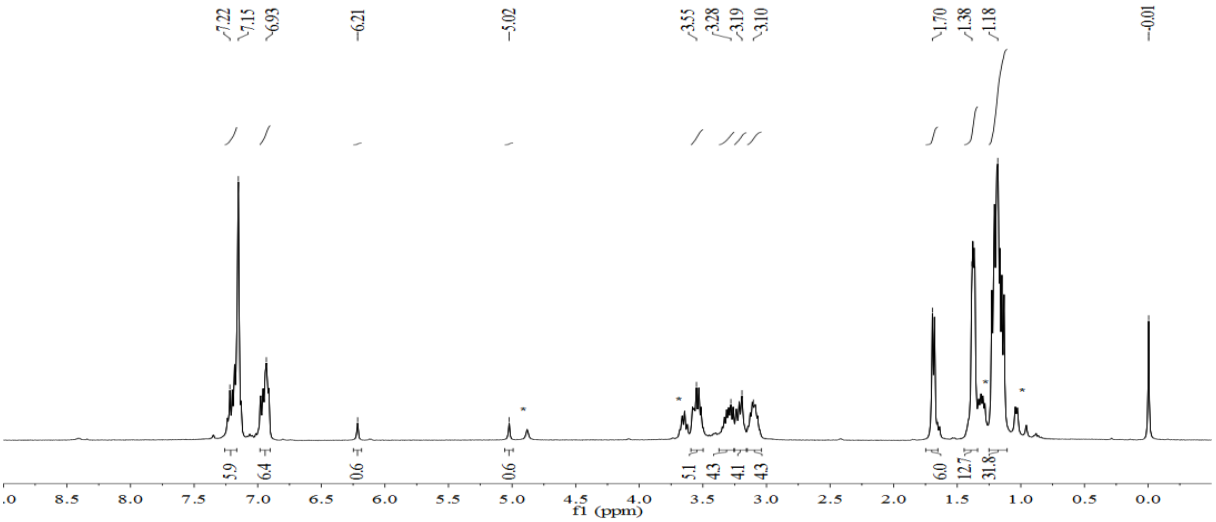

Figure S24. ^{1}H NMR spectrum of **9** in C_6D_6. *Small amount of impurity.

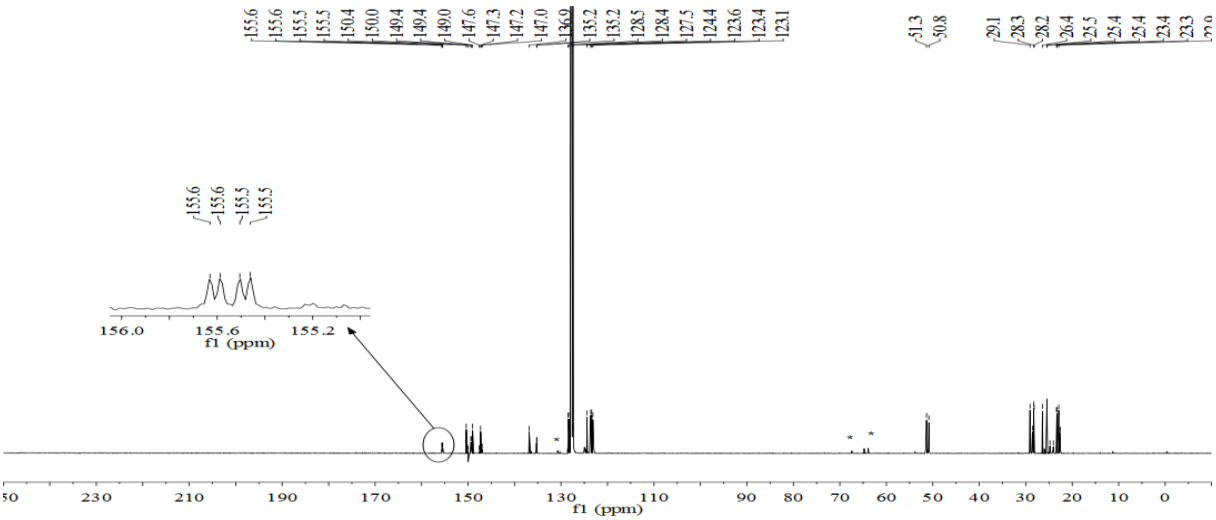

Figure S25. ^{13}C{^{1}H} NMR spectrum of **9** in C_6D_6. *Small amount of impurity.

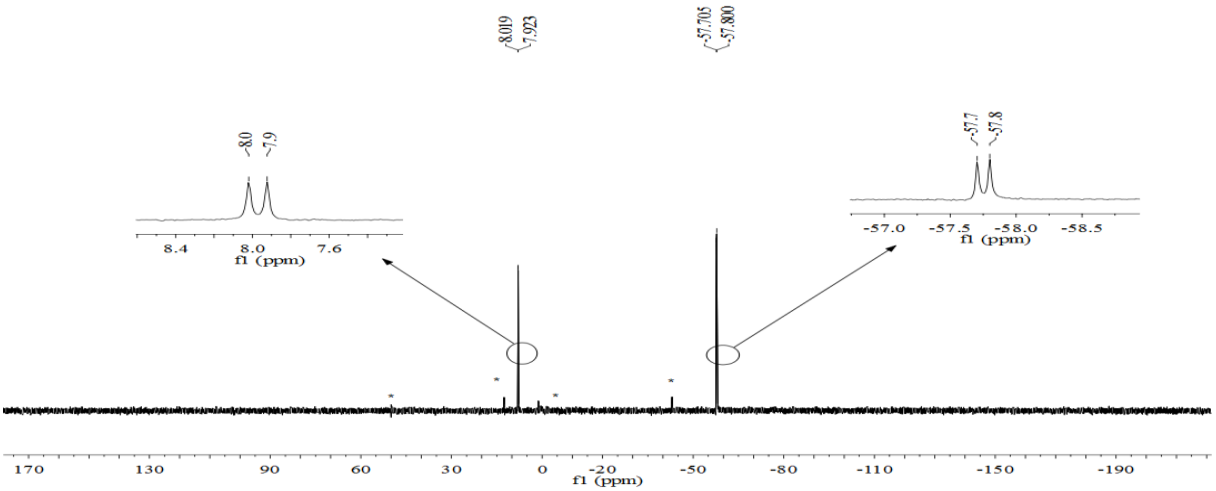

Figure S26. $^{31}P\{^{1}H\}$ NMR spectrum of **9** in C_6D_6. *Small amount of impurity.

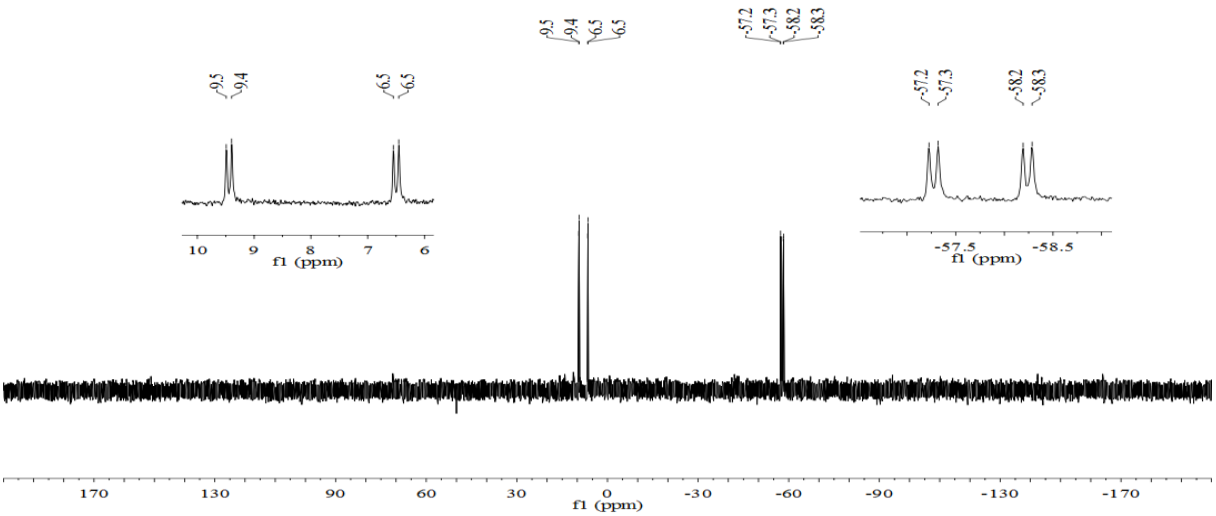

Figure S27. ^{31}P NMR spectrum of **9** in C_6D_6.

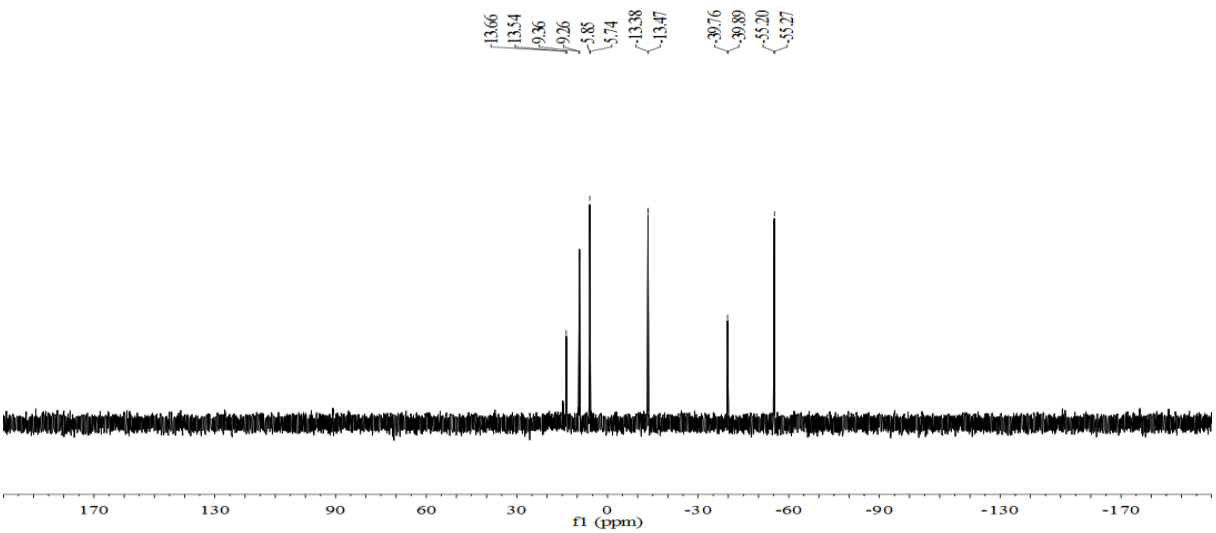

Figure S28. $^{31}P\{^{1}H\}$ NMR spectrum of the mixture of **1** and 3 equivalent of H_2O in THF.

Preparation of 8b: MeOH (2.0 equivalent) in THF (1 mL) was added to a stirred solution of **1** (86.8 mg, 0.10 mmol) in THF (3 mL). After stirring for 4 hours at 60 °C, the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* to afford **8b**'as yellow powder (66.7 mg, 0.074 mmol, 74.2% yield). Only characteristic ^{1}H NMR and ^{31}P NMR data is provided because of the presence of two isomer in the isolated product. Yellow crystals were obtained from a saturated hexane/THF solution via slow evaporation. M. P. > 250 °C ^{1}H NMR (C_6D_6, 400 MHz): *cis*-isomer: δ = 5.30 (dd, 1 H, $^{1}J_{PH}$ = 140.4 Hz, P*H*, $^{3}J_{PH}$ = 13.2 Hz, *P*CP*H*), *trans*-isomer: δ = 4.81 (dd, 1 H, $^{1}J_{PH}$ = 158.4 Hz, P*H*, $^{3}J_{PH}$ = 2.4 Hz, *P*CP*H*); ^{31}P NMR (C_6D_6, 161.9 MHz) *cis*-isomer: δ = 169.9 (m, $^{2}J_{PP}$ = 23.3 Hz, $^{3}J_{PH}$ = 7.6 Hz), 6.3 (dd, $^{2}J_{PP}$ = 23.3 Hz, $^{1}J_{PH}$ = 140.4 Hz), *trans*-isomer: δ = 178.1 (m, $^{2}J_{PH}$ = 7.1 Hz), 16.1 (d, $^{1}J_{PH}$ = 158.4 Hz). IR (solid): 2163.6 cm^{-1} (b, PH).

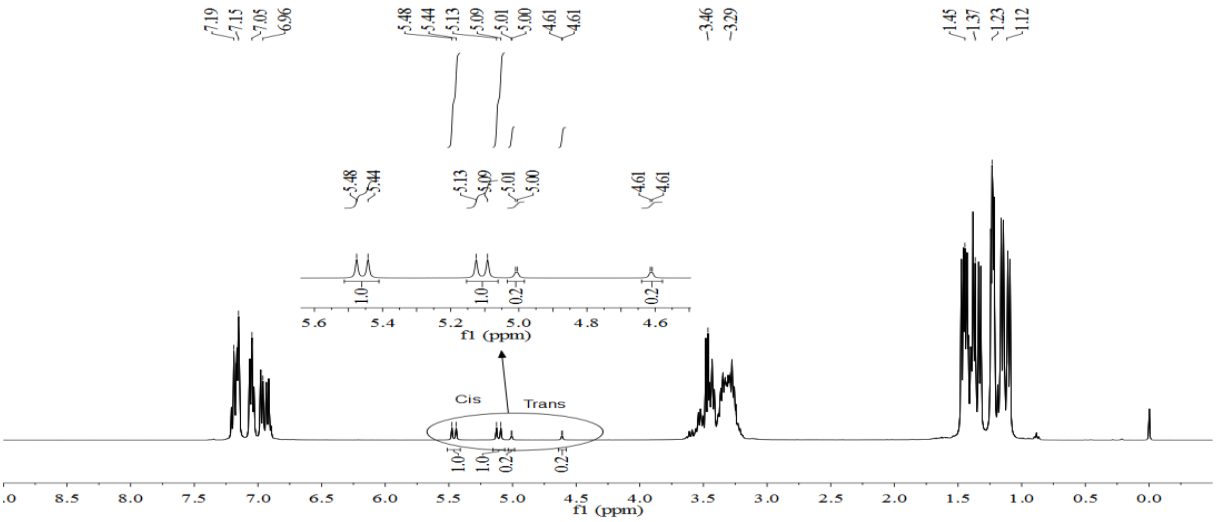

Figure S29. ^{1}H NMR spectrum of **8b** in C_6D_6.

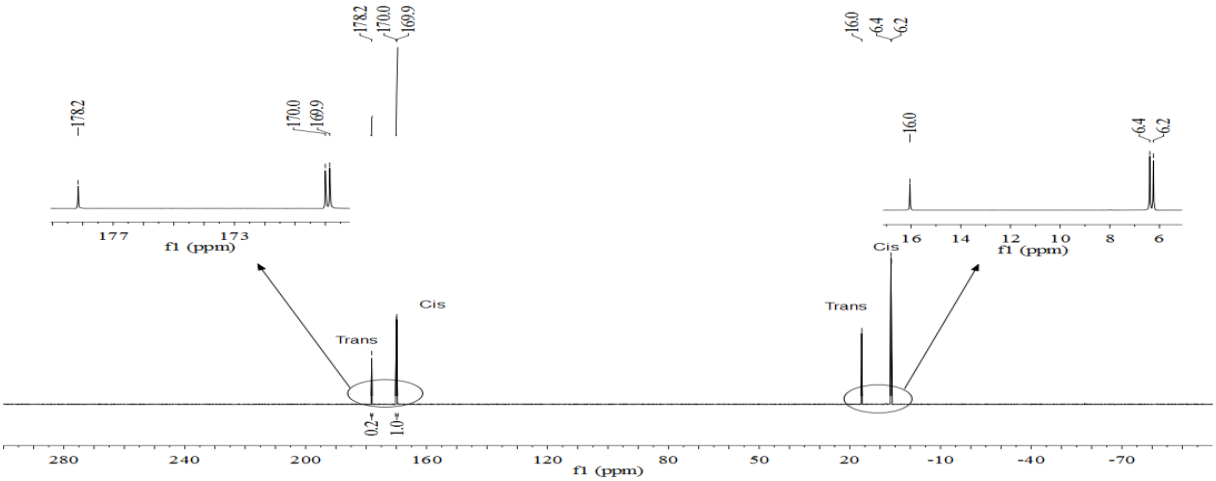

Figure S30. ^{31}P{^{1}H} NMR spectrum of **8b** in C_6D_6.

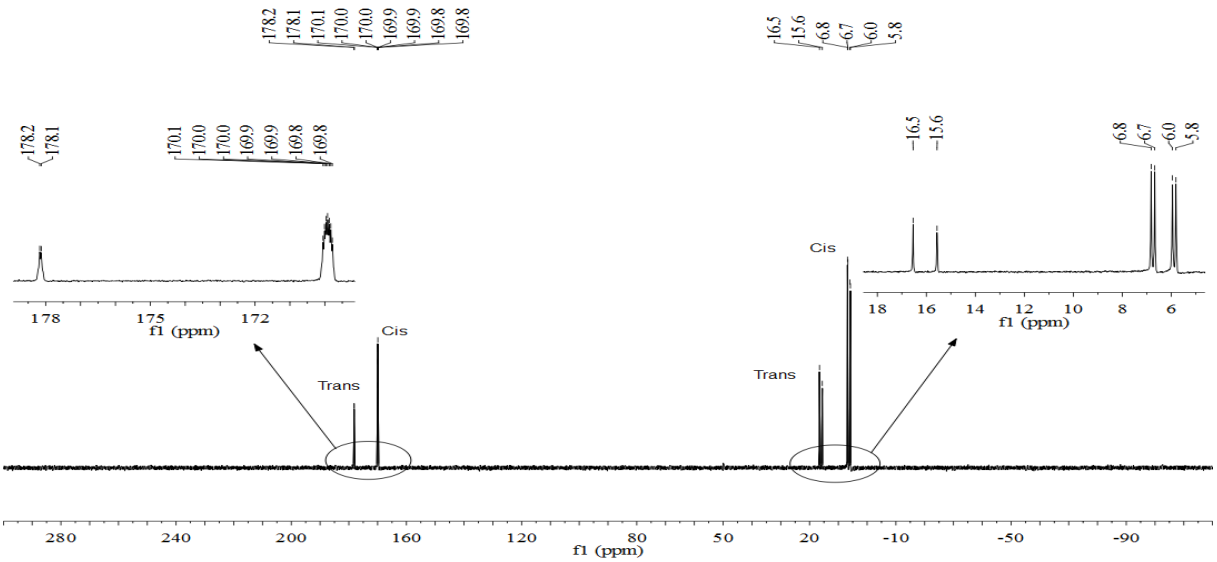

Figure S31. ^{31}P NMR spectrum of **8b** in C_6D_6.

Preparation of 8c: PhOH (1.0 equivalent) was added to a stirred solution of **1** (86.8 mg, 0.10 mmol) in THF (3 mL). After stirring for 12 hours at room temperature, the solvent was removed under reduced pressure. The remaining solid was washed with cold acetonitrile and dried *in vacuo* to afford **8c** as yellow powder (72.6 mg, 0.076 mmol, 75.5% yield). Yellow crystals were obtained from a saturated hexane/THF solution via slow evaporation. Only characteristic ^{1}H NMR and ^{31}P NMR data is provided because of the presence of two isomer in the isolated product. M. P. = 230 °C (Decomposition). ^{1}H NMR (C_6D_6, 400 MHz): *cis*-isomer: δ = 5.66 (dd, 1 H, $^{1}J_{PH}$ = 150.8 Hz, P*H*, $^{3}J_{PH}$ = 7.6 Hz, *P*CP*H*), *trans*-isomer δ = 5.02 (d, 1 H, $^{1}J_{PH}$ = 152.0 Hz, P*H*); ^{31}P NMR (C_6D_6, 161.9 MHz) *cis*-isomer: δ = 182.1 (dd, $^{2}J_{PP}$ = 27.0 Hz, $^{3}J_{PH}$ = 7.6 Hz), 18.9 (dd, $^{2}J_{PP}$ = 27.0 Hz, $^{1}J_{PH}$ = 150.8 Hz), *trans*-isomer: δ = 181.7 (m, $^{2}J_{PP}$ = 3.2 Hz), 32.2 (m, $^{2}J_{PP}$ = 3.2 Hz, $^{1}J_{PH}$ = 152.0 Hz). IR (solid): 2156.4 cm^{-1} (s, PH).

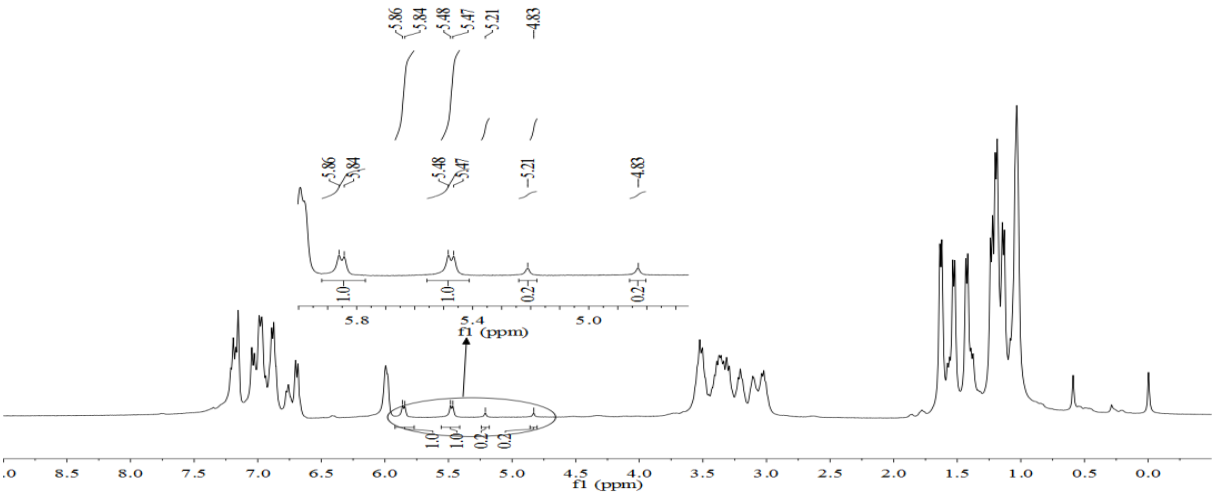

Figure S32. ^{1}H NMR spectrum of **8c** in C_6D_6.

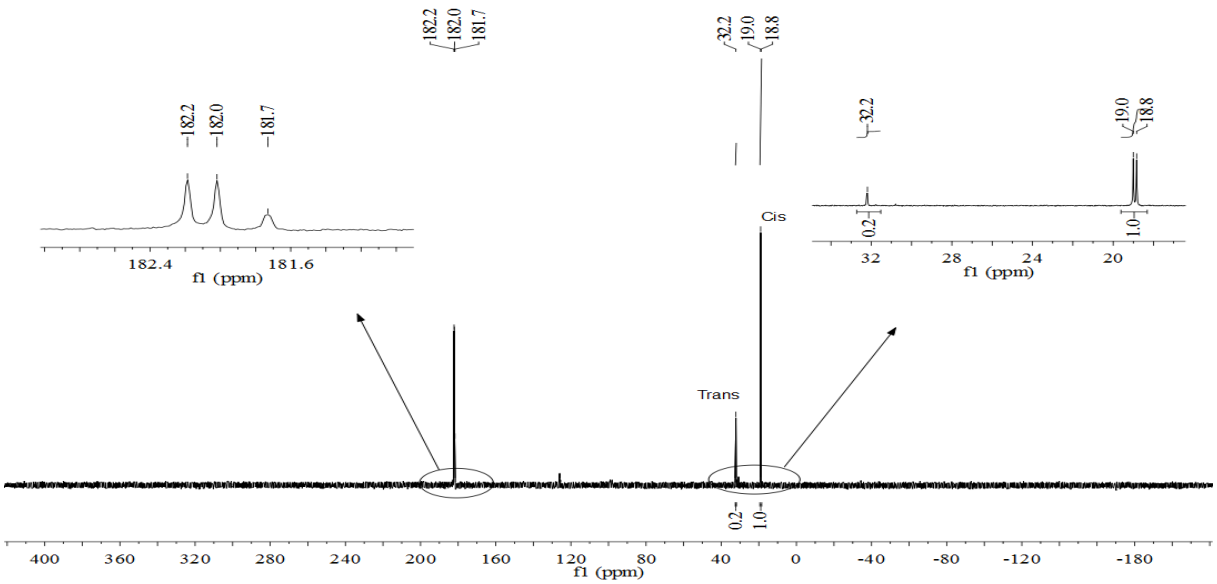

Figure S33. $^{31}P\{^{1}H\}$ NMR spectrum of **8c** in C_6D_6.

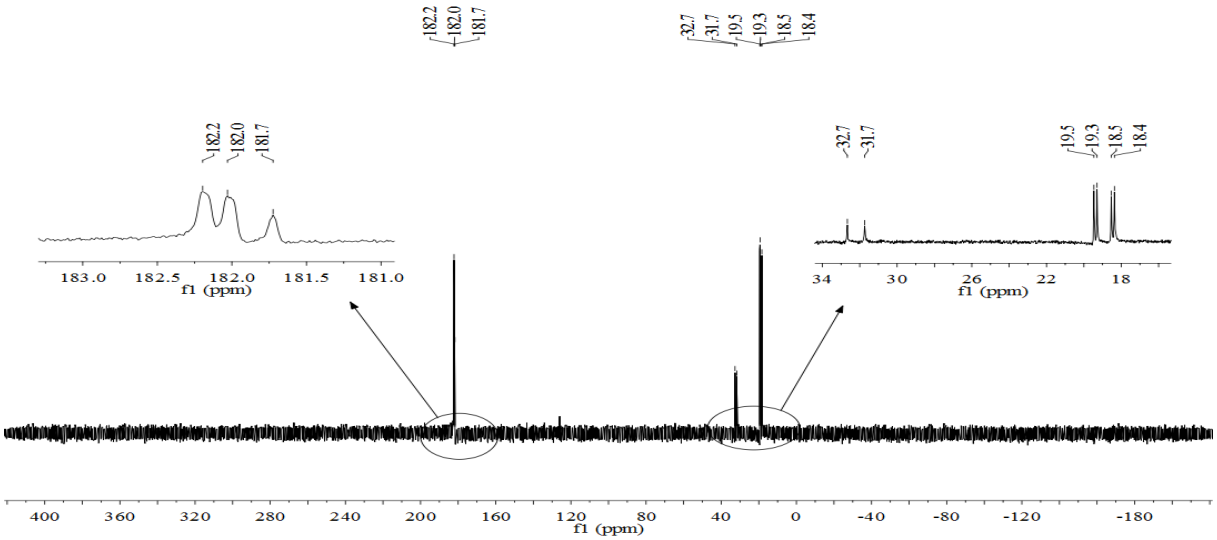

Figure S34. ^{31}P NMR spectrum of **8c** in C_6D_6.

Preparation of 10: PhOH (3.0 equivalent) was added to a stirred solution of **1** (86.8 mg, 0.10 mmol) in acetonitrile (3 mL). After stirring for 12 hours at room temperature, the solvent was removed under reduced pressure. The remaining solid was washed with hexane and dried *in vacuo* to afford **10** as orange powder (104.9 mg, 0.091 mmol, 91.3% yield). Orange crystals were obtained from a saturated C_6D_6 solution via slow evaporation. M. P. = > 250 °C. ^{1}H NMR (CD_2Cl_2, 400 MHz): δ = 13.4 (s, 2 H, PhO–HOPh), 7.35 (m, 4 H, $C_{ar}H$), 7.09 (m, 14 H, $C_{ar}H$), 6.86 (m, 6 H, $C_{ar}H$), 6.60 (m, 6 H, $C_{ar}H$), 4.91 (dd, 1 H, $^{1}J_{PH}$ = 183.2 Hz, P*H*; $^{3}J_{PH}$ = 21.2 Hz, *P*CP*H*), 4.05 (m, 8 H, CH_2), 2.84 (m, 8 H, $CHMe_2$), 1.24 (m, 24 H, CH_3) 1.06 (m, 24 H, CH_3); $^{13}C\{^{1}H\}$ NMR (CD_2Cl_2, 100.5 MHz): δ =162.1 (t, $^{2}J_{PC}$ = 10.8 Hz, PC*C*), 161.6 (C_{ar}), 147.3

(C_{ar}), 147.0 (C_{ar}), 130.7 (C_{ar}), 128.9 (C_{ar}), 125.4 (C_{ar}), 125.2 (C_{ar}), 122.3 (C_{ar}), 121.8 (dd, $^{1}J_{PC}$ = 47.4 Hz, $^{1}J_{PC}$ = 5.1 Hz, P*C*PH), 116.8 (C_{ar}), 115.9 (C_{ar}), 51.4 (s, N*C*H$_2$), 28.8, 28.8, 25.2, 25.1, 23.3, 23.2; ^{31}P NMR (CD_2Cl_2, 161.9 MHz) δ = 436.2 (dd, $^{2}J_{PP}$ = 67.5 Hz, $^{3}J_{PH}$ = 21.0 Hz), 10.2 (dd, $^{2}J_{PP}$ = 67.5 Hz, $^{1}J_{PH}$ = 182.8 Hz). UV/Vis (CH_2Cl_2, λ (nm) ε ($M^{-1}cm^{-1}$)): 266.9 (19012), 325.7 (8079), 483.1 (22400).

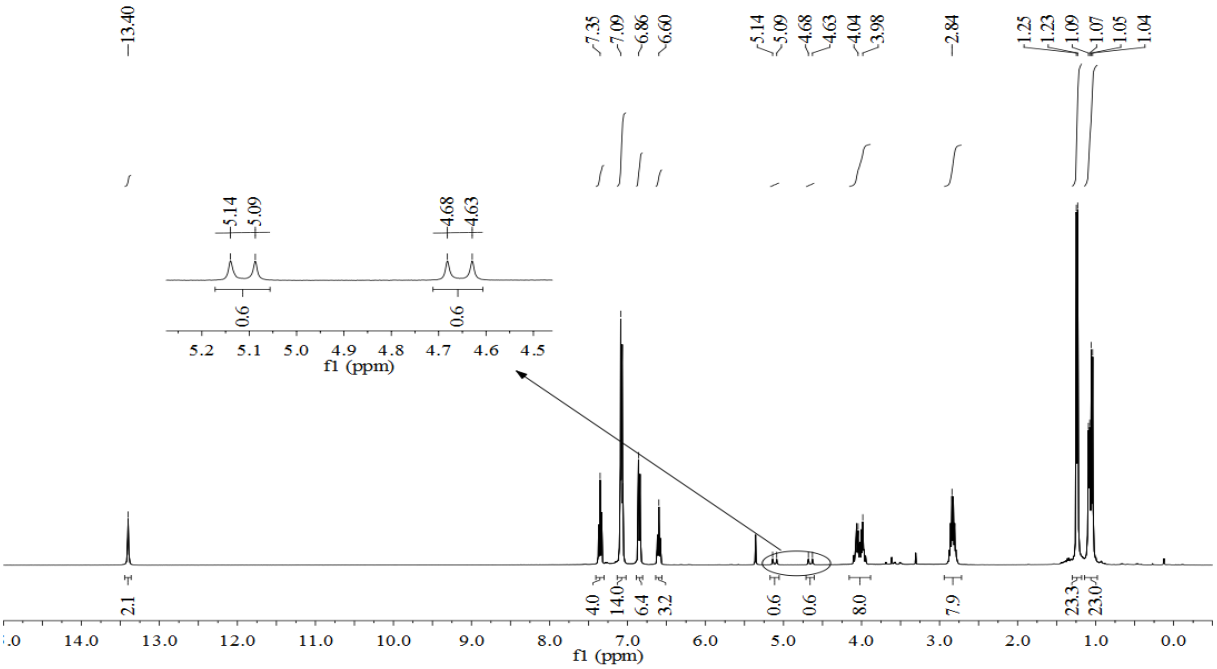

Figure S35. ^{1}H NMR spectrum of **10** in CD_2Cl_2.

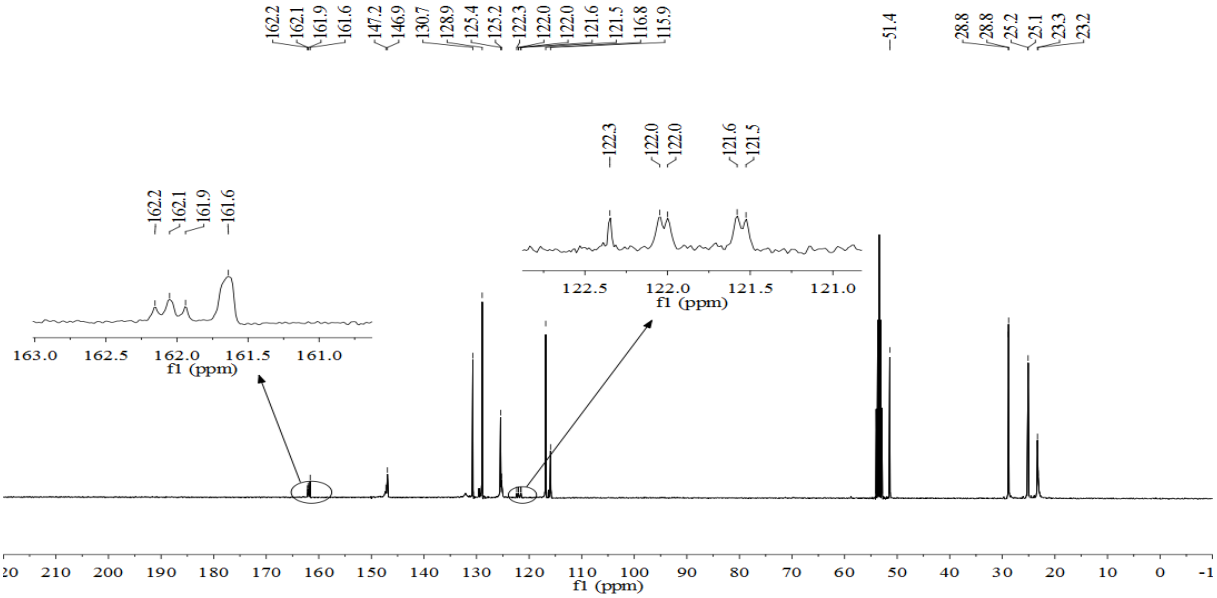

Figure S36. ^{13}C{^{1}H} NMR spectrum of **10** in CD_2Cl_2.

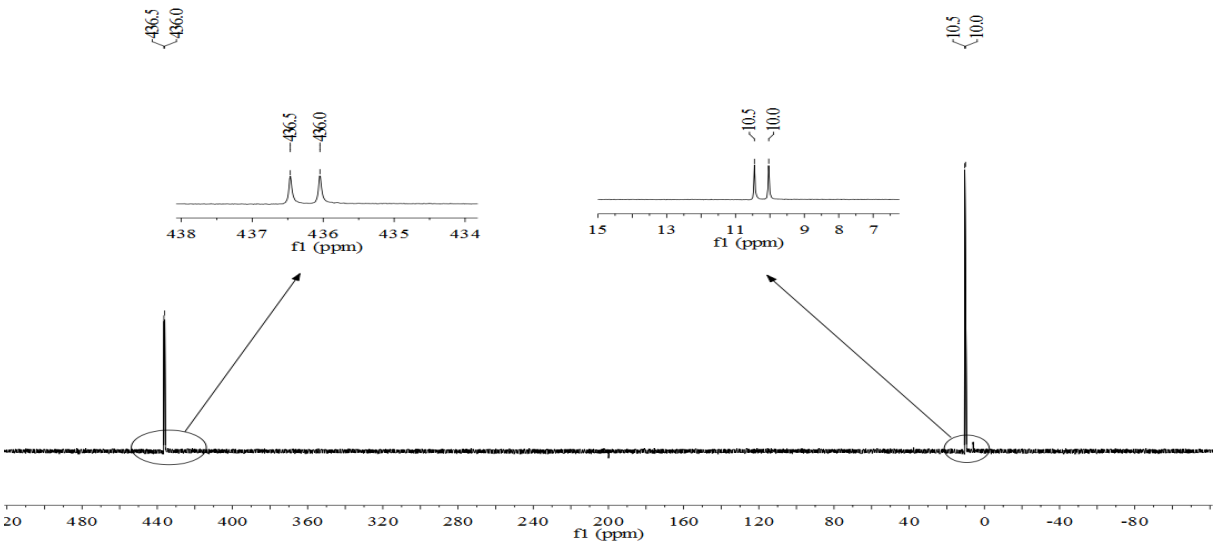

Figure S37. $^{31}P\{^{1}H\}$ NMR spectrum of **10** in CD_2Cl_2.

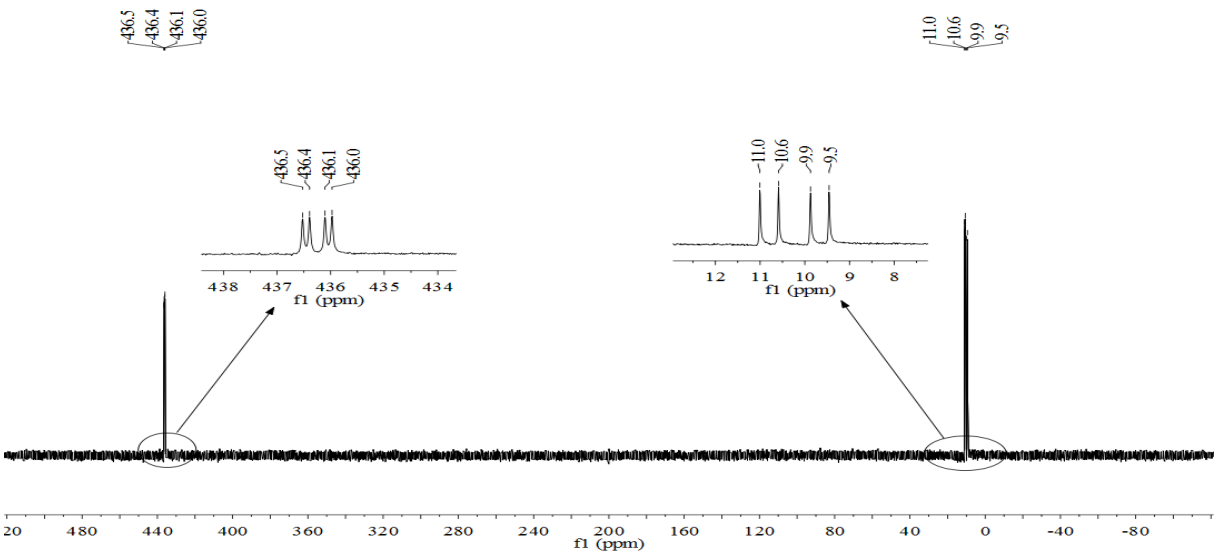

Figure S38. ^{31}P NMR spectrum of **10** in CD_2Cl_2.

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 1988878-1988885.

Table S1. The summary of crystal data and structure refinement

Compounds	**2**	**3**	**6**	**7**
CCDC	1988881	1988878	1988880	1988882

Empirical formula	$C_{64}H_{82}N_4P_2$	$C_{124}H_{161}FN_{12}P_4$	$C_{256}H_{334}N_{26}P_8$	$C_{63}H_{82}F_3N_5P_2$
Formula weight	969.27	1962.52	4023.23	1028.27
Temperature/K	150.00(10)	149.97(10)	150.00(10)	235.01(10)
Crystal system	orthorhombic	monoclinic	monoclinic	orthorhombic
Space group	$P2_12_12_1$	$P2_1/n$	$P2_1/c$	$Pca2_1$
a/Å	12.5962(2)	19.9039(3)	26.2082(9)	22.9944(4)
b/Å	13.0948(2)	16.3725(2)	21.2732(9)	13.1476(2)
c/Å	34.8018(4)	38.5734(5)	22.2484(8)	19.4279(3)
α/°	90	90	90	90
β/°	90	93.9800(10)	95.906(3)	90
γ/°	90	90	90	90
Volume/Å^3	5740.37(14)	12539.9(3)	12338.4(8)	5873.47(16)
Z	4	4	2	4
ρ_{calc}g/cm^3	1.122	1.040	1.083	1.163
μ/mm^{-1}	0.994	0.936	0.953	1.079
F(000)	2096.0	4232.0	4344.0	2208.0
Crystal size/mm^3	0.23 × 0.22 × 0.19	0.1 × 0.09 × 0.08	0.1 × 0.08 × 0.06	0.08 × 0.08 × 0.06
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.212 to 146.786	5.148 to 148.668	5.362 to 148.892	6.724 to 145.338
Index ranges	$-15 \le h \le 9$, $-15 \le k \le 16$, $-43 \le l \le 29$	$-22 \le h \le 24$, $-13 \le k \le 19$, $-47 \le l \le 48$	$-31 \le h \le 26$, $-26 \le k \le 15$, $-27 \le l \le 27$	$-26 \le h \le 28$, $-15 \le k \le 16$, $-20 \le l \le 23$
Reflections collected	14864	72764	73158	22695
Independent reflections	9701 [R_{int} = 0.0235, R_{sigma} = 0.0345]	24562 [R_{int} = 0.0320, R_{sigma} = 0.0368]	24449 [R_{int} = 0.0674, R_{sigma} = 0.0982]	9212 [R_{int} = 0.0239, R_{sigma} = 0.0277]
Data/restraints/parameters	9701/0/647	24562/62/1331	24449/13/1340	9212/25/688
Goodness-of-fit on F^2	1.033	1.054	1.006	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0371, wR_2 = 0.0934	R_1 = 0.0753, wR_2 = 0.1981	R_1 = 0.0639, wR_2 = 0.1536	R_1 = 0.0424, wR_2 = 0.1129
Final R indexes [all data]	R_1 = 0.0405, wR_2 = 0.0960	R_1 = 0.0844, wR_2 = 0.2033	R_1 = 0.1228, wR_2 = 0.1739	R_1 = 0.0482, wR_2 = 0.1182
Largest diff. peak/hole / e Å^{-3}	0.54/-0.32	0.60/-0.83	0.32/-0.29	0.44/-0.29
Flack parameter	-0.003(8)			0.027(9)

Continued

Compounds	**8b**	**8c**	**9**	**10**
CCDC	1988879	1988883	1988884	1988885
Empirical formula	$C_{57}H_{80}N_4OP_2$	$C_{62}H_{82}N_4OP_2$	$C_{56}H_{78}N_4OP_2$	$C_{77}H_{97}N_4O_3P_2$
Formula weight	899.19	961.25	885.16	1191.54
Temperature/K	150.00(10)	150.00(10)	150.00(10)	150.00(10)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	P-1

a/Å	12.42330(10)	12.71500(10)	14.36670(10)	13.3039(3)
b/Å	33.6427(3)	22.9346(2)	12.03320(10)	22.5743(7)
c/Å	12.62960(10)	21.8186(2)	15.31190(10)	26.5944(6)
α/°	90	90	90	67.479(2)
β/°	94.2270(10)	99.4350(10)	96.6110(10)	80.235(2)
γ/°	90	90	90	81.533(2)
Volume/Å^3	5264.23(8)	6276.52(10)	2629.48(3)	7241.3(3)
Z	4	4	2	4
ρ_{calc}g/cm^3	1.135	1.017	1.118	1.093
μ/mm^{-1}	1.059	0.917	1.053	0.903
F(000)	1952.0	2080.0	960.0	2564.0
Crystal size/mm^3	0.16 × 0.12 × 0.11	0.3 × 0.05 × 0.05	0.11 × 0.1 × 0.06	0.15 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.254 to 148.406	5.632 to 148.284	7.992 to 148.242	6.77 to 147.52
Index ranges	-14 ≤ h ≤ 15, -41 ≤ k ≤ 27, -13 ≤ l ≤ 15	-15 ≤ h ≤ 15, -15 ≤ k ≤ 27, -27 ≤ l ≤ 25	-17 ≤ h ≤ 17, -7 ≤ k ≤ 14, -18 ≤ l ≤ 19	-14 ≤ h ≤ 16, -27 ≤ k ≤ 28, -15 ≤ l ≤ 33
Reflections collected	33317	36570	14672	47833
Independent reflections	10457 [R_{int} = 0.0284, R_{sigma} = 0.0279]	12416 [R_{int} = 0.0296, R_{sigma} = 0.0318]	5174 [R_{int} = 0.0302, R_{sigma} = 0.0298]	28103 [R_{int} = 0.0240, R_{sigma} = 0.0359]
Data/restraints/parameters	10457/0/622	12416/2/662	5174/0/445	28103/93/1617
Goodness-of-fit on F^2	1.016	1.060	1.054	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0385, wR_2 = 0.0978	R_1 = 0.0461, wR_2 = 0.1268	R_1 = 0.0422, wR_2 = 0.1088	R_1 = 0.0531, wR_2 = 0.1373
Final R indexes [all data]	R_1 = 0.0408, wR_2 = 0.0995	R_1 = 0.0507, wR_2 = 0.1303	R_1 = 0.0446, wR_2 = 0.1105	R_1 = 0.0687, wR_2 = 0.1498
Largest diff. peak/hole / e Å^{-3}	0.55/-0.30	0.73/-0.83	0.40/-0.32	1.01/-0.63
Flack parameter				

S3. Theoretical Details

Calculations were carried out Gaussian 09 package[S2] except the IBO analysis (see below). Geometry optimizations were performed using the M06-2X functional.[S3] The Def2-SVP basis set was used for all the atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide the thermal corrections of Gibbs free energy. Transition states were submitted to intrinsic reaction coordinate (IRC) calculations to determine two corresponding minima.

The single-point energy calculations were performed at the M06-2X/Def2-TZVP level of theory for solution-phase (THF). The gas-phase geometry was used for all the solution phase calculations. The SMD method was used with the corresponding solvent, while the Bondi radii were chosen as the atomic radii to define the molecular cavity. The Gibbs energy corrections from frequency calculations were added to the single-point energies to obtain the Gibbs free energies in solution, respectively. All the solution-phase free energies reported in the paper correspond to the reference state of 1 mol/L, 298K. NBO calculations were carried out using NBO 6.0 program[S4] at the M06-2X/TZVP//M06-2X/Def2-SVP level of theory. Optimized structures were visualized by the IBOview program.[S5] IBOs were carried out using ORCA programS5 at the PBE/Def2-TZVP//M06-2X/Def2-SVP level of theory.

Table S2. Calculated energies of model compounds for this paper.

Species	Thermal Corrections of Gibbs Free Energies (Enthalpies are given in parentheses) (Hartree)	Solvation Energies (Hartree)
1	1.114525	-3081.28057495
PhC≡CH	0.080445	-308.380589409
IN1A	1.217700	-3389.67234431
TS1A	1.215322	-3389.64261491
2	1.213241	-3389.68830476
PhOH	0.077095	-307.469568762
IN1B	1.218028	-3388.76982602
TS1B	1.212330	-3388.74006809
8c	1.215825	-3388.77638003

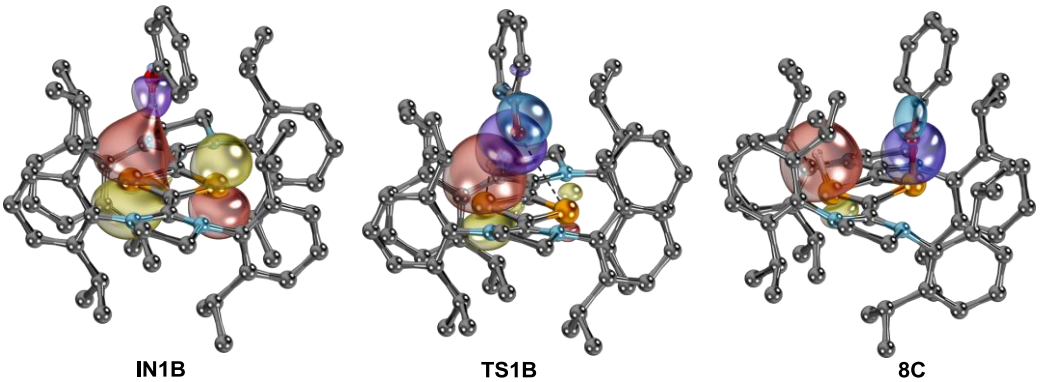

Figure S39. Depiction of selected IBOs (O–H σ-electrons and π-electrons at P) for **IN1C**, **TS1C**, and **IN2C**.

1

P	-0.24116	1.332062	-0.16447
P	-0.16075	-1.42216	-0.40666
N	-3.50467	-1.27975	-0.26805
N	-3.57614	0.892995	0.146343
N	3.186724	-1.02523	-0.46476
N	3.113946	1.181388	-0.34678
C	0.951004	-0.00466	-0.34429

C	-4.92616	-0.94656	-0.26091	C	1.605478	4.97146	-1.34822
H	-5.31461	-0.90204	-1.29484	H	1.503802	5.336576	0.768034
C	-2.73815	-0.15209	-0.11471	H	1.720838	4.32344	-3.39783
C	2.344516	0.046154	-0.38307	H	1.217216	5.958017	-1.60818
C	-4.93324	0.428959	0.40593	C	2.406634	2.950477	1.799227
H	-5.67647	1.115628	-0.02061	H	2.249705	1.861398	1.826375
C	-1.34949	-0.08718	-0.21289	C	2.591051	1.768956	-3.15924
C	4.518206	0.864293	-0.58978	H	2.947683	0.826874	-2.7169
H	5.179477	1.473943	0.039238	C	1.338361	3.579485	2.691932
C	4.571721	-0.62384	-0.2496	H	1.491934	4.663316	2.81402
H	5.254763	-1.19443	-0.89261	H	0.337168	3.406426	2.268549
H	-5.11836	0.354203	1.492707	H	1.377623	3.128887	3.694957
H	-5.50848	-1.69463	0.292831	C	3.814021	3.250075	2.325342
H	4.78034	1.049909	-1.64726	H	3.920059	2.913629	3.367653
H	4.868409	-0.79039	0.801714	H	4.584557	2.74692	1.723848
C	-3.13712	2.192694	0.542293	H	4.01586	4.331985	2.292117
C	-2.90644	3.153788	-0.46108	C	3.645579	2.241806	-4.16404
C	-2.89533	2.4559	1.90044	H	4.608098	2.450342	-3.67317
C	-2.51914	4.433254	-0.05909	H	3.809138	1.477895	-4.93895
C	-2.5193	3.754713	2.257942	H	3.322808	3.165659	-4.66773
C	-2.34664	4.736961	1.289448	C	1.261087	1.448382	-3.84947
H	-2.32306	5.198974	-0.80984	H	0.51149	1.141106	-3.10522
H	-2.32874	3.989425	3.307852	H	0.871571	2.327866	-4.38659
H	-2.04341	5.743265	1.584465	H	1.392821	0.635518	-4.58101
C	-3.04644	-2.41813	-1.00483	C	2.890548	-2.20116	2.19231
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C	-2.23851	-4.67968	-1.04695	H	1.985512	-1.3129	-2.64263
C	-2.51496	-3.4537	-3.10695	C	4.087909	-2.73138	2.986526
C	-2.16863	-4.62217	-2.43518	H	3.918868	-3.77362	3.298204
H	-1.93248	-5.58991	-0.52937	H	5.012149	-2.71009	2.389598
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H	-1.82444	-5.49115	-2.99925	C	1.613337	-2.19886	3.040244
C	2.768332	-2.386	-0.35944	H	0.762979	-1.82496	2.44946
C	2.40322	-3.06467	-1.53895	H	1.370036	-3.21342	3.392927
C	2.679564	-2.98465	0.907319	H	1.744975	-1.55712	3.924565
C	2.027378	-4.40432	-1.42717	C	1.368941	-2.94139	-3.85347
C	2.312342	-4.33292	0.969383	H	0.380771	-3.05836	-3.38316
C	2.000928	-5.03806	-0.18681	H	1.26106	-2.28512	-4.72993
H	1.725357	-4.95823	-2.31617	H	1.709858	-3.92297	-4.21896
H	2.237976	-4.82636	1.941143	C	3.750815	-2.19535	-3.49435
H	1.704176	-6.08648	-0.12043	H	3.698495	-1.62819	-4.4366
C	2.596604	2.470808	-0.68906	H	4.448386	-1.67232	-2.82435
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C	-3.01019	2.772019	-1.93018
H	-2.65682	1.731446	-2.00138
C	-2.94367	1.364845	2.957188
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H	-1.24084	2.055247	4.137756
H	-1.57447	0.311886	4.27931
H	-0.80966	0.962277	2.794451
C	-4.00026	1.654295	4.027049
H	-3.7572	2.57478	4.579801
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C	-1.93362	-0.47579	-3.76653
H	-1.53637	-1.15442	-4.53831
H	-2.12092	0.50245	-4.23754
H	-1.1666	-0.35389	-2.9865
C	-4.02182	-4.20325	1.716498
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C	3.195305	1.149962	0.000332
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IN1A

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H	0.997142	-3.84514	-1.51223
C	4.810483	-4.11304	-0.86063
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C	-1.14547	2.675704	-4.34111
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C	-5.42618	4.463216	1.374687
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H	0.389854	2.005952	5.588857
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H	3.346378	4.766884	0.999242
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C	-3.89075	-1.93156	-2.17467
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H	-5.59096	-1.15827	-3.24722
C	-0.27504	-2.14658	-3.47896
H	0.080577	-2.22544	-2.44443
C	-4.71733	-2.23844	-0.93792
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C	0.000772	-3.47109	-4.19981
H	1.079388	-3.69013	-4.21005
H	-0.51708	-4.31302	-3.71439
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H	0.27314	-0.05197	-3.60762
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H	-5.88681	-1.19573	0.569545
H	-4.61093	-0.19441	-0.19989
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C	-5.76243	-3.32105	-1.22802
H	-5.2973	-4.2411	-1.6127
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C	0.348595	-2.27936	4.303302
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C	-2.02041	-1.93838	4.576479
H	1.355771	-2.27554	4.723302
H	-0.58333	-1.76731	6.17423
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C	1.391297	-2.75834	2.054373

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C	-3.6403	-2.11648	2.632108
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H	3.255221	-1.76836	1.555712
H	1.979276	-0.66458	2.152387
H	2.871909	-1.72303	3.288197
C	2.018804	-4.14351	2.24769
H	2.853357	-4.28442	1.541941
H	2.410885	-4.24891	3.271851
H	1.290803	-4.95345	2.087683
C	-4.26064	-3.50037	2.412729
H	-5.25396	-3.40797	1.946022
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H	-4.84017	-1.69609	4.417391

TS1A

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C	1.830752	-0.9669	-0.65478
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C	2.844071	-1.89946	-0.97836
C	2.51584	-3.27305	-1.09059
C	4.19063	-1.52692	-1.19271
C	3.489038	-4.22028	-1.38633
H	1.4778	-3.57966	-0.94176
C	5.154916	-2.48413	-1.48591
H	4.465371	-0.47402	-1.1276
C	4.817126	-3.83586	-1.58239
H	3.207317	-5.27236	-1.46538
H	6.188283	-2.17007	-1.64405
H	5.579898	-4.58099	-1.81098
C	-4.07414	3.383082	-0.50851
C	-2.83376	3.579747	-1.14561
C	-2.68019	3.407259	-2.53332
C	-3.80446	3.055186	-3.28381
C	-5.03641	2.852126	-2.6702
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H	-3.70909	2.905598	-4.36022
H	-5.90004	2.557239	-3.26928
H	-6.1364	2.836991	-0.81952
C	-1.32081	3.567385	-3.1904
H	-0.56502	3.405114	-2.40546
C	-4.23763	3.519876	0.995326
H	-3.29473	3.91554	1.401257
C	-1.07409	2.531478	-4.28903
H	-0.02334	2.567096	-4.61239
H	-1.29411	1.51632	-3.92587
H	-1.6967	2.726083	-5.17617
C	-1.15063	4.992397	-3.73043
H	-0.14886	5.129628	-4.16449
H	-1.89532	5.192761	-4.51655
H	-1.29263	5.74323	-2.93963
C	-5.3457	4.513183	1.355885
H	-5.39004	4.659393	2.445399
H	-5.17824	5.491025	0.880884
H	-6.33086	4.146465	1.030182
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H	-3.65445	1.458893	1.440143
H	-4.56886	2.27264	2.74588
H	-5.41718	1.709548	1.285583
C	0.112793	2.592093	3.497305
C	0.615585	2.931422	2.230069
C	1.920038	2.570371	1.826219
C	2.728041	1.905714	2.750322
C	2.262664	1.610367	4.030413
C	0.967315	1.947249	4.398175
H	3.73496	1.599555	2.468399
H	2.912657	1.090286	4.7362

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H	1.78002	4.970383	0.395252
H	3.464806	4.705633	0.90666
C	3.641194	2.061031	0.029088
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C	-4.51638	-1.28452	-3.38988
H	-1.64879	-1.15524	-5.20642
H	-4.0393	-0.54122	-5.35348
H	-5.56472	-0.98393	-3.45292
C	-0.32747	-2.35439	-3.12286
H	-0.06119	-2.29063	-2.05768
C	-4.98465	-2.10806	-1.05018
H	-4.40913	-2.56603	-0.23338
C	-0.08033	-3.79129	-3.59732
H	0.98346	-4.05188	-3.48943
H	-0.67343	-4.51799	-3.02318
H	-0.35706	-3.89896	-4.65786
C	0.588245	-1.38211	-3.86395
H	1.636778	-1.60581	-3.61663
H	0.478924	-1.46704	-4.95676
H	0.379618	-0.34262	-3.5691
C	-5.51704	-0.77345	-0.52104
H	-6.13208	-0.93843	0.378236
H	-4.68762	-0.09779	-0.26466
H	-6.14406	-0.26825	-1.27265
C	-6.12504	-3.06468	-1.4099
H	-5.73995	-4.03036	-1.76987
H	-6.76496	-3.25115	-0.53414
H	-6.7595	-2.64139	-2.20385
C	-2.44768	-2.19171	3.273591
C	-1.33028	-2.60184	2.510129
C	-0.03945	-2.66376	3.064467
C	0.11072	-2.36973	4.424512
C	-0.98004	-2.00069	5.199322
C	-2.24485	-1.89895	4.622782
H	1.103356	-2.41778	4.875375
H	-0.84594	-1.7728	6.258399
H	-3.08489	-1.57468	5.237371
C	1.174391	-3.01286	2.221306
H	0.885153	-2.88535	1.166062
C	-3.82875	-2.07027	2.644715
H	-3.68622	-1.61845	1.650344
C	2.349676	-2.06492	2.474794
H	3.156327	-2.27466	1.755971
H	2.041687	-1.01562	2.353116
H	2.762432	-2.19652	3.487494
C	1.602611	-4.4691	2.438772
H	2.434827	-4.72711	1.766091
H	1.942572	-4.616	3.476174
H	0.776802	-5.17362	2.260727
C	-4.48496	-3.44426	2.466958
H	-5.46112	-3.34445	1.966378
H	-3.86233	-4.11882	1.863466
H	-4.64902	-3.92126	3.44572
C	-4.76527	-1.14037	3.414414
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H	-5.05928	-1.56601	4.386268

2

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C	-1.23135	5.168696	0.036508
H	-2.12601	5.808018	0.061049

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H	-2.34366	-4.99757	-1.28778
C	-1.6724	-4.43012	0.73316
H	-2.08737	-5.08941	1.508062
H	-0.48909	5.634497	-0.63601
H	0.202476	5.593439	1.662257
H	-3.64658	-4.40353	-0.22413
H	-0.68028	-4.81797	0.434209
H	-0.84825	0.300051	-1.95018
C	1.957237	-0.86724	-0.28087
C	1.060426	-0.34352	0.361048
C	2.931098	-1.5628	-1.07138
C	2.955625	-2.96904	-1.06085
C	3.825464	-0.8751	-1.9084
C	3.846279	-3.66491	-1.87324
H	2.255234	-3.50666	-0.41809
C	4.714607	-1.57787	-2.71634
H	3.801817	0.214236	-1.92694
C	4.727212	-2.973	-2.70526
H	3.849695	-4.75612	-1.85996
H	5.399793	-1.0307	-3.36568
H	5.422085	-3.52085	-3.34322
C	-3.96398	3.344154	-0.54188
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C	-3.70168	2.922607	-3.30418
C	-4.93519	2.75123	-2.68311
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H	-3.60929	2.732345	-4.37419
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H	-6.03138	2.803893	-0.83212
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H	-0.46496	3.198094	-2.4478
C	-4.12233	3.508733	0.959138
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H	0.04298	2.448293	-4.69613
H	-1.2743	1.415793	-4.07387
H	-1.61899	2.709497	-5.25197
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H	0.025645	4.984097	-4.12208
H	-1.71733	5.138986	-4.46586
H	-1.08907	5.581813	-2.86443
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H	-5.2518	4.689373	2.395073
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H	-6.20289	4.176613	0.986248
C	-4.38906	2.16103	1.638898
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C	0.124042	2.616585	3.569133
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C	1.956594	2.574642	1.926463
C	2.757544	1.942625	2.880214
C	2.277582	1.679309	4.161386
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H	3.773869	1.64577	2.623562
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H	0.599122	1.778538	5.499847
C	2.47718	2.878093	0.52825
H	1.709365	2.517623	-0.17857
C	-1.32935	2.876222	3.928945
H	-1.86661	3.1021	2.99482
C	2.669499	4.384392	0.31191
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H	1.731003	4.938568	0.427009
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H	4.048763	2.329368	-0.84807
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H	3.703427	1.074499	0.373255
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H	-0.99036	4.976013	4.463333
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H	-0.96702	3.854294	5.837737
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C	-1.74647	-2.07404	-3.12799
C	-2.18793	-1.45388	-4.29908
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H	-1.47558	-1.229	-5.09294
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H	-5.48663	-1.03315	-3.58105
C	-0.28414	-2.44425	-2.92162
H	-0.03331	-2.18702	-1.87774
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H	-4.51221	-2.5424	-0.2667

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H	-0.33231	-4.25278	-4.13305
C	0.675321	-1.67121	-3.82419
H	1.713521	-1.9226	-3.56084
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C	-5.5777	-0.74697	-0.66041
H	-6.23831	-0.87496	0.212147
H	-4.74943	-0.07539	-0.38813
H	-6.15965	-0.25328	-1.45482
C	-6.18215	-3.05795	-1.50371
H	-5.79628	-4.0436	-1.80388
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H	-6.76549	-2.65665	-2.347
C	-2.53915	-2.19712	3.29625
C	-1.42651	-2.69545	2.578909
C	-0.16752	-2.83768	3.190553
C	-0.04549	-2.52958	4.550044
C	-1.13408	-2.06413	5.274247
C	-2.36567	-1.88826	4.646265
H	0.923737	-2.63809	5.039953
H	-1.02372	-1.82087	6.332521
H	-3.20373	-1.49486	5.222297
C	1.045558	-3.29326	2.39968
H	0.811547	-3.11863	1.33684
C	-3.89286	-2.01823	2.62413
H	-3.70001	-1.61899	1.616038
C	2.296603	-2.47577	2.735633
H	3.09259	-2.68517	2.004263
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H	2.687159	-2.73456	3.732209
C	1.313079	-4.78898	2.608697
H	2.162446	-5.12219	1.992101
H	1.56284	-4.9853	3.663164
H	0.437894	-5.40447	2.35613
C	-4.62018	-3.36031	2.486123
H	-5.57178	-3.23261	1.945925
H	-4.01461	-4.09654	1.941002
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C	-4.79284	-1.00877	3.334913
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H	0.550603	0.90502	-2.1422
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C	0.95479	-0.01954	-0.25561
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C	-2.73933	-0.1294	0.002773
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H	5.187097	1.41834	0.169522
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H	5.250862	-1.25218	-0.76637
H	-5.13687	0.447799	1.549161
H	-5.50538	-1.64986	0.449377
H	4.810479	1.006504	-1.52652
H	4.839857	-0.83318	0.922302
H	-0.95897	-1.04213	2.095692
O	-1.20522	-1.15453	3.037257
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C	-2.4875	-3.51881	-2.89253
C	-2.16181	-4.6734	-2.18687
H	-1.99561	-5.6019	-0.25341
H	-2.37871	-3.5003	-3.97953
H	-1.80856	-5.55669	-2.72227
C	2.771268	-2.4324	-0.47492
C	2.359715	-2.91354	-1.73705
C	2.766362	-3.25255	0.666448
C	1.994476	-4.25584	-1.83879
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C	2.029209	-5.09507	-0.7285
H	1.655342	-4.65185	-2.7954
H	2.400568	-5.25312	1.381471
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C	2.623314	2.445945	-0.57748
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C	1.928952	4.054047	-2.22571
C	1.643005	4.96303	-1.21284
H	1.569133	5.313725	0.907503
H	1.754832	4.332103	-3.26775
H	1.256967	5.952991	-1.46263
C	2.462192	2.931513	1.915254
H	2.358419	1.837045	1.938248
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H	3.005136	0.844502	-2.63235
C	1.364287	3.512269	2.806212
H	1.50457	4.592164	2.972033
H	0.374259	3.349981	2.353514
H	1.380711	3.019734	3.790367
C	3.853184	3.291364	2.44784
H	3.962682	2.974348	3.496397
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C	3.709402	2.292661	-4.0393
H	4.661131	2.500773	-3.52781
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C	1.329183	1.470244	-3.78047
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H	1.486423	0.683471	-4.53528
C	3.097657	-2.72256	2.050002
H	3.043277	-1.62259	2.006662
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H	4.568586	-4.23279	2.580684
H	5.275116	-2.8318	1.75507
H	4.756919	-2.69553	3.459382
C	2.068235	-3.17931	3.086833
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H	2.226665	-2.65391	4.040658
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H	0.304593	-2.68875	-3.51742
H	1.128738	-1.70001	-4.75427
H	1.632612	-3.38124	-4.50219
C	3.649265	-1.72984	-3.5589
H	3.569976	-1.00959	-4.38837
H	4.35522	-1.31951	-2.82145
H	4.077783	-2.66359	-3.95479
C	-2.7804	-3.59878	1.422104
H	-2.77703	-2.5547	1.764333
C	-3.21291	-1.11116	-3.0287
H	-3.58569	-0.33561	-2.34442
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H	-2.49988	1.520678	-2.01269
C	-3.21525	1.824561	2.966831
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C	-2.01496	3.307719	-3.03906
H	-1.94975	2.774189	-3.9992
H	-2.40631	4.314998	-3.25137
H	-0.99895	3.398089	-2.62401
C	-4.34381	2.432886	-2.61862
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C	-4.49716	2.162086	3.735874
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C	-4.29451	-1.34344	-4.08819
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H	-1.14737	-0.43143	-2.88826
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H	-1.53015	-4.08042	3.125449
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C	-0.21163	-1.23477	5.175236
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H	-1.07883	-1.79914	5.521007
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H	0.802312	-1.24321	7.071255
H	2.778035	0.025139	6.231302

TS1B

P	-0.25909	1.311829	0.147211
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H	-5.3422	-0.86258	-1.24728
C	-2.7658	-0.16899	-0.14742
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C	4.544105	-0.76237	-0.11642
H	5.235893	-1.26671	-0.80431
H	-4.99568	0.13789	1.635553
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H	4.859299	1.07691	-1.27414
H	4.79188	-1.06664	0.913842
H	-0.45503	0.747287	1.546016
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C	-3.05204	2.705892	1.718913
C	-2.67488	4.351435	-0.53
C	-2.73314	4.061473	1.863442
C	-2.55717	4.877488	0.754609
H	-2.48967	4.996473	-1.38837
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8C

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H	2.197206	-0.86456	6.586631

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